SUPPLEMENTARY MATERIAL

Atalantums H-K from the peels of *Atalantia monophylla* and their Cytotoxicity

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ABSTRACT

Four new benzoyletryamines, atalantums H-K (1-4) and seven known compounds were isolated from the peels of *Atalantia monophylla*. All compounds were tested for cytotoxicity against HeLa, HCT116 and MCF-7 cell lines, as well as normal cells (Vero cells). Compound 5 showed cytotoxicity against HeLa, HCT116 and MCF-7 cell lines with IC$_{50}$ values ranging from 16-25 µg/mL but was inactive against Vero cells. Compound 6 also showed interesting results as compound 5 with IC$_{50}$ values ranging from 15-18 µg/mL and an IC$_{50}$ value of 80.20 µg/mL against Vero cells. This means compounds 5 and 6 can be used as lead compounds for anticancer agents.

KEYWORDS *Atalantia monophylla*; atalantum; benzoyletryamine
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Table S1. $^1$H NMR spectroscopic data of compounds 1–4 (CDCl$_3$, δ in ppm)

| position | 1              | 2              | 3              | 4              |
|----------|----------------|----------------|----------------|----------------|
| 1        | 4.54, d (4.0)  | 4.57, d (8.0)  | 4.57, d (8.0)  | 4.53, d (8.0)  |
| 2        | 5.76, t (8.0)  | 5.83, t (8.0)  | 5.83, t (8.0)  | 5.72, t (4.0)  |
| 4        | 4.27, dd (8.0, 4.0) | 5.42, dd (8.0, 4.0) | 5.42, dd (8.0, 4.0) | 4.89, dd (8.0, 4.0) |
| 5        | 1.58, m        | 1.78, m        | 1.79, m        | 1.78, m        |
| 6        | 3.64, t (8.0)  | 3.35 dd (8.0, 4.0) | 3.35 dd (8.0, 4.0) | 4.12, t (8.0)  |
| 8        | 1.10, s        | 1.09, s        | 1.08, s        | 1.13, s        |
| 9        | 1.09, s        | 1.07, s        | 1.07, s        | 1.12, s        |
| 10       | 1.72, s        | 1.73, s        | 1.73, s        | 1.70, s        |
| 2', 6'   | 6.84, d (8.0)  | 6.85, d (8.0)  | 6.84, d (8.0)  | 6.83, d (8.0)  |
| 3', 5'   | 7.12, d (8.0)  | 7.13, d (8.0)  | 7.13, d (8.0)  | 7.11, d (8.0)  |
| 7'       | 2.84, t (8.0)  | 2.86, t (8.0)  | 2.86, t (8.0)  | 2.83, t (8.0)  |
| 8'       | 3.65, m        | 3.68, m        | 3.67, m        | 3.63, m        |
| 2'', 6'' | 7.66, d (8.0)  | 7.69, d (8.0)  | 7.69, d (8.0)  | 7.68, d (8.0)  |
| 3'', 5'' | 7.38, t (8.0)  | 7.41, t (8.0)  | 7.40, t (8.0)  | 7.37, t (8.0)  |
| 4''      | 7.46, t (8.0)  | 7.47, t (8.0)  | 7.48, t (8.0)  | 7.44, t (8.0)  |
| 2'''     | -              | 2.28, t (8.0)  | 2.28, t (8.0)  | 2.30, t (8.0)  |
| 3'''     | -              | 1.60, m        | 1.60, m        | 1.60, m        |
| CH$_2$ (4'''-15''') | -          | 1.25, m        | 1.25, m        | 1.24, m        |
| CH$_3$ (14'''' or 16''''' ) | -          | 0.87, t (8.0)  | 0.87, t (8.0)  | 0.86, t (8.0)  |
| 7-OMe    | 3.20, s        | 3.18, s        | 3.18, s        | 3.20, s        |
| NH       | 6.39, br t (8.0) | 6.16, br t (8.0) | 6.19, br t (8.0) | 6.40, br t (8.0) |
Table S2. $^{13}$C NMR spectroscopic data of compounds 1–4 (CDCl$_3$, $\delta$ in ppm)

| position | 1   | 2   | 3   | 4   |
|----------|-----|-----|-----|-----|
| 1        | 64.0| 64.5| 64.5| 64.6|
| 2        | 120.3| 124.5| 124.5| 121.7|
| 3        | 141.3| 137.3| 137.3| 141.3|
| 4        | 76.5| 77.1| 77.1| 74.6|
| 5        | 35.1| 34.4| 34.4| 34.7|
| 6        | 76.9| 74.1| 74.1| 75.5|
| 7        | 76.5| 77.1| 77.1| 76.3|
| 8        | 19.6| 20.5| 20.5| 22.2|
| 9        | 18.7| 19.5| 19.5| 20.6|
| 10       | 11.8| 12.6| 12.6| 12.3|
| 7-OMe    | 48.6| 49.3| 49.3| 49.8|
| 1'       | 156.8| 157.5| 157.5| 157.5|
| 2', 6'   | 114.3| 115.1, 115.2| 115.1, 115.2| 115.0|
| 3', 5'   | 129.2| 129.9| 129.9| 129.8|
| 4'       | 130.4| 131.2| 131.2| 131.0|
| 7'       | 34.1| 34.9| 34.9| 35.3|
| 8'       | 40.6| 41.4| 41.4| 41.4|
| 9'       | 167.2| 167.6| 167.6| 167.5|
| 1''      | 133.9| 134.8| 134.8| 134.7|
| 2'', 6'' | 126.2| 126.9| 126.9| 126.9|
| 3'', 5'' | 128.0| 128.7| 128.7| 128.6|
| 4''      | 130.8| 131.5| 131.5| 131.4|
| 1'''     | -    | 172.9| 172.9| 173.7|
| 2'''     | -    | 34.8| 34.8| 34.9|
| 3'''     | -    | 25.1| 25.1| 25.1|
| 4''''-13''' | - | 32.1, 29.8-29.3, | 32.1, 29.8-29.3, | 32.0, 29.7-29.3, |
| or 4''''-15''' | 22.8 | 22.8 | 22.8 | 22.7 |
| 14''' or 16''' | - | 14.3 | 14.3 | 14.2 |

Table S3. Cytotoxicity of isolated compounds (IC$_{50}$, $\mu$g/mL)

| compound | Hela cells | HCT116 cells | MCF-7 cells | Vero cells |
|----------|------------|--------------|-------------|------------|
| 5        | 19.09 ± 2.83 | 16.02 ±0.10 | 25.89 ± 3.49 | > 100      |
| 6        | 15.03 ± 0.46 | 16.65 ± 3.21 | 18.33 ± 0.31 | 80.20 ± 4.35 |
| 7        | 22.44 ± 2.59 | 19.75 ± 0.44 | 16.18 ± 1.10 | 25.20 ± 1.41 |
| 10       | 20.06 ± 2.42 | 35.74 ± 2.02 | 24.44 ± 1.12 | 50.60 ± 2.19 |
| The other | inactive | inactive | inactive | inactive |
| cisplatin | 6.65 ± 0.12 | 4.93 ± 0.77 | 10.42 ± 0.85 | 6.55 ± 0.81 |
Figure S1. The HMBC correlations of compound 1.

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