Supplementary materials

Histone deacetylase inhibitors and antioxidants from the root of *Gluta usitata*

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**Supplemental files**

**Figure S1.** Mass spectrum of glutacoside (1).

**Figure S2.** $^1$H-NMR spectrum of glutacoside (1).

**Figure S3.** $^{13}$C-NMR spectrum of glutacoside (1).

**Figure S4.** DEPT spectrum of glutacoside (1).

**Figure S5.** COSY spectrum of glutacoside (1).

**Figure S6.** NOESY spectrum of glutacoside (1).

**Figure S7.** HMQC spectrum of glutacoside (1).

**Figure S8.** HMBC spectrum of glutacoside (1).

**Figure S9.** IR spectrum of glutacoside (1).

**Figure S10.** Mass spectrum of 3,4,5-trimethoxyphenol-1-O-β-D-glucopyranoside (2).

**Figure S11.** $^1$H-NMR spectrum of 3,4,5-trimethoxyphenol-1-O-β-D-glucopyranoside (2).

**Figure S12.** $^{13}$C-NMR spectrum of 3,4,5-trimethoxyphenol-1-O-β-D-glucopyranoside (2).

**Figure S13.** IR spectrum of 3,4,5-trimethoxyphenol-1-O-β-D-glucopyranoside (2).

**Figure S14.** $^1$H-NMR spectrum of β-sitosterol-3-O-β-D-glucoside (3).

**Figure S15.** $^{13}$C-NMR spectrum of β-sitosterol-3-O-β-D-glucoside (3).

**Figure S16.** IR spectrum of β-sitosterol-3-O-β-D-glucoside (3)

**Figure S17.** $^1$H-NMR spectrum of fisetin (7).

**Figure S18.** $^{13}$C-NMR spectrum of fisetin (7).

**Figure S19.** IR spectrum of fisetin (7).

**Table S1.** % HDAC Inhibitory activity at 1 µM of the compounds.

**Table S2.** % HDAC Inhibitory activity at 100 µM of the compounds.
Figure S1. Mass spectrum of glutacoside (1).

Figure S2. $^1$H-NMR spectrum of glutacoside (1).
Figure S3. $^{13}$C-NMR spectrum of glutacoside (1).

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Figure S10. Mass spectrum of 3,4,5-trimethoxyphenol-1-β-D-glucopyranoside (2).
Figure S11. $^1$H-NMR spectrum of 3,4,5-trimethoxyphenol-1-$O$-$\beta$-$D$-glucopyranoside (2).

Figure S12. $^{13}$C-NMR spectrum of 3,4,5-trimethoxyphenol-1-$O$-$\beta$-$D$-glucopyranoside (2).
Figure S13. IR spectrum of 3,4,5-trimethoxyphenol-1-O-β-D-glucopyranoside (2).

Figure S14. $^1$H-NMR spectrum of β-sitosterol-3-O-β-D-glucoside (3).
Figure S15. $^{13}$C-NMR spectrum of $\beta$-sitosterol-3-$O$-$\beta$-D-glucoside (3).

Figure S16. IR spectrum of $\beta$-sitosterol-3-$O$-$\beta$-D-glucoside (3)
Figure S17. $^1$H-NMR spectrum of fisetin (7).

Figure S18. $^{13}$C-NMR spectrum of fisetin (7).
Figure S19. IR spectrum of fisetin (7).

HDAC inhibitory activities

Relative Fluorescence Unit (RFU) = (reading sample/ reading No inhibitor) x 100

% HDAC inhibition = [ (RFU interference – RFU test) / RFU interference] x 100

Table S1. % HDAC Inhibitory activity at 1 μM of the compounds.

| Compound | HDAC inhibition test | Interference test | (%) HDAC inhibition |
|----------|----------------------|-------------------|-------------------|
|          | Reading | RFU    | Reading | RFU    |                |
| No inhibitor | 59035.2 | 100.0  | 56084.1 | 100    | 0.0            |
| DMSO     | 43960.1 | 100.0  | 59898.0 | 106.8  | 6.4            |
| TSA      | 4064.7  | 9.2    | 39748.0 | 70.9   | 87.0           |
| 1        | 38979.7 | 88.7   | 51643.0 | 92.1   | 3.7            |
| 2        | 40933.4 | 93.1   | 55034.0 | 98.1   | 5.1            |
| 3        | 42564.2 | 96.8   | 55246.0 | 98.5   | 1.7            |
| 4        | 33265.9 | 75.7   | 54812.0 | 91.5   | 17.3           |
| 5        | 37298.3 | 84.8   | 54785.0 | 97.7   | 13.1           |
| 6        | 37298.3 | 84.8   | 54285.0 | 96.8   | 12.3           |
| 7        | 33553.0 | 76.3   | 52356.0 | 93.4   | 18.2           |
Table S2. % HDAC Inhibitory activity at 100 µM of the compounds.

| Compound | HDAC inhibition test | Interference test | (%) HDAC inhibition |
|----------|----------------------|-------------------|---------------------|
|          | Reading | RFU | Reading | RFU |     |
| No inhibitor | 59035.2 | 100.0 | 49084.1 | 100.0 | 0.0 |
| DMSO     | 53465.0 | 90.6 | 50987.0 | 103.9 | 12.8 |
| TSA      | 1868.6  | 3.2  | 39748.0 | 81.0 | 96.1 |
| 1        | 39140.0 | 57.2 | 30820.0 | 171.2 | 64.6 |
| 2        | 21537.0 | 31.5 | 13969.0 | 77.6 | 59.4 |
| 3        | 42692.0 | 62.4 | 30617.0 | 170.0 | 63.3 |
| 4        | 6106.0  | 10.3 | 34432.0 | 70.1 | 85.3 |
| 5        | 7910.6  | 13.4 | 34246.0 | 69.8 | 80.8 |
| 6        | 7943.0  | 11.6 | 8063.0  | 44.8 | 74.1 |
| 7        | 5011.9  | 8.5  | 35465.0 | 72.3 | 88.3 |