SUPPLEMENTARY MATERIAL

Three new acyltyramines from *Anisodus luridus* Link et Otto (Solanaceae)

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Abstract

Three new acyltyramines, N-[2-(4-hydroxyphenyl)ethyl]hentriacontanamide (1), N-[2-(4-hydroxyphenyl)ethyl]nonacosanamide (2) and N-[2-(4-hydroxyphenyl)ethyl]heneicosanamide (3) have been isolated from n-hexane extract of leaves of *Anisodus luridus* (Solanaceae). Successive extraction of defatted leaves of *A. luridus* with methanol afforded a residue on removal of solvent under reduced pressure. Residue was partitioned by means of chloroform and *n*-butanol. Chromatographic resolution of *n*-BuOH extract afforded six known compounds, apigenin (4), luteolin (5), quercetin (6), quercetin-3-O-α-L-rhamnoside (7), kaempferol 3-O-α-rhamnoside (8) and quercetin 3-O-α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside (9). The structures of the isolated compounds were assigned with the help of spectroscopic techniques. This is the first report of isolation of these compounds from this plant.

Keywords: *Anisodus luridus*, acyltyramines, leaves, Solanaceae
Table S1: \(^1^H\) and \(^{13}C\) NMR spectral data of compounds 1, 2 and 3

| Position | \(\delta_C\) | \(\delta_H\)            | \(\delta_C\) | \(\delta_H\)            | \(\delta_C\) | \(\delta_H\)            |
|----------|-----------|-------------------------|-----------|-------------------------|-----------|-------------------------|
| 2        | 34.6      | 2.11 t (7.5, 8 Hz)      | 34.6      | 2.11 t (10, 5 Hz)       | 34.6      | 2.11 t (7.5 Hz)         |
| 3        | 25.7      | 1.25 br s               | 25.7      | 1.57 t (5, 10 Hz)       | 25.7      | 1.25 br s               |
| 21       | *         | *                       | *         | *                       | 13.9      | 0.88 t (6.5, 7 Hz)      |
| 29       | *         | *                       | 13.9      | 0.88 t (5 Hz)           | -         | -                       |
| 31       | 13.9      | 0.88 t (7 Hz)           | -         | -                       | -         | -                       |
| 1'       | 40.6      | 3.47 q (6.5 Hz)         | 40.6      | 3.43 q (6.6 Hz)         | 40.8      | 3.47 q (6.5 Hz)         |
| 2'       | 36.6      | 2.74 t (7 Hz)           | 36.6      | 2.71 t (5, 10 Hz)       | 36.6      | 2.74 t (7, 6.5 Hz)      |
| 3'       | 129.7     | -                       | 129.7     | -                       | 129.7     | -                       |
| 4',8'    | 129.6     | 7.05 d (8 Hz)           | 129.6     | 7.02 d (10 Hz)          | 129.6     | 7.05 d (8.5 Hz)         |
| 5',7'    | 115.3     | 6.78 d (8 Hz)           | 115.3     | 6.77 d (10 Hz)          | 115.3     | 6.78 d (8.5 Hz)         |
| 6'       | 155.2     | -                       | 155.2     | -                       | 155.2     | -                       |

* Chemical shifts for methylenes of respective acyltyramine are shown in experimental section for the sake of proper depiction of data in the table.

# \(\delta_H\) (500 MHz, CDCl\(_3\)) ; \(\delta_C\) (125 MHz, CDCl\(_3\) / CDCl\(_3\)-CD\(_3\)OD)
Table S2: $^1$H NMR spectral data of compounds 4-9

| Position | Compound 4' | Compound 5 | Compound 6 | Compound 7 | Compound 8 | Compound 9 |
|----------|-------------|------------|------------|------------|------------|------------|
|          | $\delta_H$  | $\delta_C$ | $\delta_H$  | $\delta_C$ | $\delta_H$  | $\delta_C$ | $\delta_H$  | $\delta_C$ | $\delta_H$  | $\delta_C$ |
| 2        | 2           | 157.3      | 164.4      | 146.4      | 157.0      | 155.9      | 156.8      |
| 3        | 6.97,       | 103.7      | 6.78,      | 103.2      | 135.4      | 134.4      | 133.3      | 133.5      |
|          | s           | s          |            |            |            |            |            |            |
| 4        | -           | 181.6      | -          | 182.0      | -          | 175.5      | -          | 172.2      | -          | 176.9      | -          | 177.6      |
| 5        | -           | 163.7      | -          | 99.1       | -          | 160.7      | -          | 161.3      | -          | 158.8      | -          | 161.4      |
| 6        | 5.88,       | 98.9       | 6.29,      | 164.2      | 6.17       | 98.2       | 6.21,      | 99.1       | 6.22       | 97.2       | 6.15,      | 99.1       |
|          | s           | d          | , d        | d          | d          | s          |            |            |            |            |            |            |
|          | 1.9         | 1.8        | 1.8        | 1.8        |            |            |            |            |            |            |            |            |
|          | Hz          | Hz         | Hz         | Hz         |            |            |            |            |            |            |            |            |
| 7        | -           | 164.6      | -          | 94.2       | -          | 164.0      | -          | 164.6      | -          | 163.1      | -          | 164.8      |
| 8        | 6.03,       | 94.0       | 6.55,      | 157.6      | 6.42       | 93.5       | 6.39,      | 94.1       | 6.39,      | 92.2       | 6.35,      | 94.6       |
|          | s           | d          | , d        | d          | d          | s          |            |            |            |            |            |            |
|          | 1.9         | 1.8        | 1.8        | 1.8        |            |            |            |            |            |            |            |            |
|          | Hz          | Hz         | Hz         | Hz         |            |            |            |            |            |            |            |            |
| 9        | -           | 157.3      | -          | 104.6      | -          | 156.4      | -          | 156.9      | -          | 156.6      | -          | 156.9      |
| 10       | -           | 103.4      | -          | 161.8      | -          | 103.2      | -          | 104.0      | -          | 103.3      | -          | 104.1      |
| 1'       | -           | 121.1      | -          | 121.8      | -          | 122.1      | -          | 121.2      | -          | 120.0      | -          | 121.9      |
| 2'       | 7.70,       | 128.4      | 7.54,      | 113.7      | 7.64       | 115.3      | 7.30,      | 115.9      | 6.95,      | 129.2      | 7.51,      | 116.5      |
|          | d          | dd         | , d        | d          | d          | s          |            |            |            |            |            |            |
|          | 8.8         | 7.5        | 2.1        | 1.9        | 7.0        |            |            |            |            |            |            |            |
|          | Hz          | Hz         | Hz         | Hz         |            |            |            |            |            |            |            |            |
| 3'       | 6.57,       | 116.0      | -          | 146.6      | -          | 144.9      | -          | 145.6      | 7.77,      | 113.9      | -          | 145.0      |
|          | d          |            |            |            |            |            |            |            | d          |            |            |            |
|          | 8.8         |            |            |            |            |            |            |            | 7.0        |            |            |            |
|          | Hz          |            |            |            |            |            |            |            | Hz         |            |            |            |
| 4'       | -           | 161.2      | -          | 150.0      | -          | 148.1      | -          | 148.5      | -          | 160.4      | -          | 148.0      |
| 5'       | 6.57,       | 116.0      | 7.00,      | 116.3      | 6.88       | 115.6      | 6.86,      | 116.1      | 7.77,      | 113.9      | 6.83,      | 115.5      |
|      |      |      |      |      |      |
|------|------|------|------|------|------|
| d,   | d,   | d,   | d,   | d,   | d,   |
| 8.8  | 7.5  | 8.7  | 8.8  | 7.0  | 9.1  |
| Hz    | Hz    | Hz    | Hz    | Hz    | Hz    |
| 6′    | 7.70, | 128.4 | 7.52, | 119.3 | 7.63  | 121.7 |
| d,   | dd,   | dd,   | d,   | d,   | d,   |
| 8.8  | 7.5  | 8.7  | 8.8  | 7.0  | 9.1  |
| Hz    | &    | &    | Hz   | Hz   | Hz   |
| 2.0  | 2.1  | 1.9  |      |      |      |
| 1″    | -    | -    | -    | -    | -    |
|      |      |      | 5.25, | 102.3 | 5.39, | 100.8 | 101.5 |
| d,   | d,   | d,   | 1.8  | 1.2  | 5    |
| Hz    | Hz    | Hz    |      |      |      |
| 2″    | -    | -    | -    | -    | -    |
|      |      |      | 3.69, | 78.8  | 4.0,  | 69.4  | 4.5,  | 74.3 |
| -    |      |      |      |      | 3.0,  |      | 3.0,  |      |
| m    |      |      | 3.10, |      |      | m    | m    |      |
| 3″    | -    | -    | -    | -    | -    |
|      |      |      | 3.69, | 78.8  | 4.0,  | 69.5  | 4.5,  | 76.7 |
| -    |      |      |      |      | 3.0,  |      | 3.0,  |      |
| m    |      |      | 3.10, |      |      | m    | m    |      |
| 4″    | -    | -    | -    | -    | -    |
|      |      |      | 3.69, | 71.7  | 4.0,  | 70.6  | 4.5,  | 70.3 |
| -    |      |      |      |      | 3.0,  |      | 3.0,  |      |
| m    |      |      | 3.10, |      |      | m    | m    |      |
| 5″    | -    | -    | -    | -    | -    |
|      |      |      | 3.69, | 70.5  | 4.0,  | 69.3  | 4.5,  | 76.1 |
| -    |      |      |      |      | 3.0,  |      | 3.0,  |      |
| m    |      |      | 3.10, |      |      | m    | m    |      |
| 6″    | -    | -    | -    | -    | -    |
|      |      |      | 0.85, | 17.9  | 0.94, | 14.9  | 4.5,  | 67.3 |
| d,   | d,   | d,   | 6.0  | 6.9  | 3.0,  |      |      |      |
| Hz    | Hz    | Hz    |      |      |      |      |      |      |
| 1''   | -   | -   | -   | -   | -   | -   | -   | -   | -   | 4.5-3.0, 101.6 m         |
| 2''   | -   | -   | -   | -   | -   | -   | -   | -   | -   | 4.5-3.0, 70.8 m          |
| 3''   | -   | -   | -   | -   | -   | -   | -   | -   | -   | 4.5-3.0, 70.6 m          |
| 4''   | -   | -   | -   | -   | -   | -   | -   | -   | -   | 4.5-3.0, 72.1 m          |
| 5''   | -   | -   | -   | -   | -   | -   | -   | -   | -   | 4.5-3.0, 68.5 m          |
| 6''   | -   | -   | -   | -   | -   | -   | -   | -   | -   | 4.5-3.0, 17.9 m          |
Figure S1: FT-IR spectra of alkyltrimines 1-3
Figure S2: $^1$H NMR spectrum of compound 1 ($N$-hentriacontanoyltyramine)

Figure S3: $^1$H NMR spectrum of compound 2 ($N$-nonacosanoyltyramine)
Figure S4: $^1$H NMR spectrum of compound 3 (N-heneicosanoyltyramine)

Figure S5: $^{13}$C NMR spectrum
Figure S6: $^1H-^1H$ COSY spectrum