



Supplementary Material

Identification of Ten New *N*-acetyldopamine Dimers from *Periostracum Cicadae*

Lu Yang^{1,2*}, Ke Zhang³ and Jin-Hui Wang^{1,2,4}

¹Key Laboratory of Forest Resources and Utilization in Xinjiang of National Forestry and Grassland Administration, Xinjiang Academy of Forestry, Urumqi 830052, China.

²Key Laboratory of Fruit tree Species Breeding and Cultivation in Xinjiang, Urumqi 830052, China.

³Key Laboratory of Xinjiang Phytomedicine Resource and Utilization, Ministry of Education, College of Pharmacy, Shihezi University, Shihezi 832002, China.

⁴College of Pharmacy, Harbin Medical University, Harbin 150081, China.

Supplementary Table S1. The detailed information of Cicadamide C1 (1)–C10 (10).

Compound	Detailed information
Cicadamide C1 (1)	White powder; MP: 180.6–181.2 °C; $[\alpha]_D^{20} +7.9^\circ$ (<i>c</i> =0.003, MeOH) IR ($\nu_{\text{KB}}^{\text{cm}^{-1}}$): 3278, 3067, 1506, 1371, 1263, 1031 UV (MeOH) $\lambda_{\text{max}}(\log \epsilon)$: 280.6 nm ¹ H NMR (600 MHz, CD ₃ OD): see Table I. ¹³ C NMR (150 MHz, CD ₃ OD): see Table I. HMBC: see Figure 2. ESI-TOF-HR-MS: <i>m/z</i> 578.2160 [M+H] ⁺ ; calcd. 578.2139 for C ₃₀ H ₃₂ N ₃ O ₉ (2 <i>S</i> ,3 <i>R</i> ,2' <i>R</i> ,3' <i>S</i>)-2-(3',4'-dihydroxyphenyl)-3-acetylamino-7-(<i>N</i> -acetyl-2-aminoethyl)-1,4-benzodioxan-2-yl)-1,4-benzodioxane
Cicadamide C2 (2)	White powder MP: 184.5–187.3 °C $[\alpha]_D^{20} +24.3^\circ$ (<i>c</i> 0.009, MeOH) IR ($\nu_{\text{KB}}^{\text{cm}^{-1}}$): 3257, 3047, 1649, 1502, 1437, 1373, 1269, 1020 UV (MeOH) $\lambda_{\text{max}}(\log \epsilon)$: 280.3 nm ¹ H NMR (600 MHz, CD ₃ OD): see Table II. ¹³ C NMR (150 MHz, CD ₃ OD): see Table II. HMBC: see Figure 2. ESI-TOF-HR-MS: <i>m/z</i> 578.2141 [M+H] ⁺ ; calcd. 578.2139 for C ₃₀ H ₃₂ N ₃ O ₉ (2 <i>R</i> ,3 <i>S</i> ,2' <i>R</i> ,3' <i>S</i>)-2-(3',4'-dihydroxyphenyl)-3-acetylamino-7-(3-acetylamino-7-(<i>N</i> -acetyl-2-aminoethyl)-1,4-benzodioxan-2-yl)-1,4-benzodioxane

Table continued on next page.....

* Corresponding author: yanglukitty127@163.com
 0030-9923/2024/0001-0047 \$ 9.00/0



Copyright 2024 by the authors. Licensee Zoological Society of Pakistan.

This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

Compound	Detailed information
Cicadamide C3 (3)	<p>White powder MP: 181.3–198.9 °C $[\alpha]_D^{20}$ -26.1° (<i>c</i> 0.03, MeOH) IR ($\nu_{\text{KB}}^{\text{cm}^{-1}}$): 3269, 3047, 1678, 1506, 1437, 1373, 1267, 1213 UV (MeOH) $\lambda_{\text{max}}(\log \epsilon)$: 280.8 nm ¹H NMR (600 MHz, CD₃OD): see Table III. ¹³C NMR (150 MHz, CD₃OD): see Table III. HMBC: see Figure 2. ESI-TOF-HR-MS: <i>m/z</i> 578.2111 [M+H]⁺; calcd. 578.2139 for C₃₀H₃₂N₃O₉ (2<i>S</i>,3<i>R</i>,2'<i>S</i>,3'<i>R</i>)-2-(3',4'-dihydroxyphenyl)-3-acetylamino-7-(3-acetylamino-6-(<i>N</i>-acetyl-2-aminoethyl)-1,4-benzodioxan-2-yl)-1,4-benzodioxane</p>
Cicadamide C4 (4)	<p>White powder MP: 179.7–182.7°C $[\alpha]_D^{20}$ +13.4° (<i>c</i> 0.006, MeOH) IR ($\nu_{\text{KB}}^{\text{cm}^{-1}}$): 3398, 3062, 1654, 1506, 1438, 1373, 1267, 1028 UV (MeOH) $\lambda_{\text{max}}(\log \epsilon)$: 280.8 nm ¹H NMR (600 MHz, CD₃OD): see Table IV. ¹³C NMR (150 MHz, CD₃OD): see Table IV. HMBC: see Figure 2. ESI-TOF-HR-MS: <i>m/z</i> 578.2114 [M+H]⁺; calcd. 578.2139 for C₃₀H₃₂N₃O₉ (2<i>R</i>,3<i>S</i>,2'<i>R</i>,3'<i>S</i>)-2-(3',4'-dihydroxyphenyl)-3-acetylamino-7-(3-acetylamino-6-(<i>N</i>-acetyl-2-aminoethyl)-1,4-benzodioxan-2-yl)-1,4-benzodioxane</p>
Cicadamide C5 (5)	<p>White powder MP: 226.3–228.7°C $[\alpha]_D^{20}$ +15.2° (<i>c</i> 0.006, MeOH) IR ($\nu_{\text{KB}}^{\text{cm}^{-1}}$): 3062, 1653, 1508, 1438, 1373, 1253, 1027 UV (MeOH) $\lambda_{\text{max}}(\log \epsilon)$: 280.8 nm ¹H NMR (600 MHz, CD₃OD): see Table V. ¹³C NMR (150 MHz, CD₃OD): see Table V. HMBC: see Figure 2. ESI-TOF-HR-MS: <i>m/z</i> 578.2144 [M+H]⁺; calcd. 578.2139 for C₃₀H₃₂N₃O₉ 2-(3',4'-dihydroxyphenyl)-3-acetylamino-6-(3-acetylamino-6-(<i>N</i>-acetyl-2-aminoethyl)-1,4-benzodioxan-2-yl)-1,4-benzodioxane</p>
Cicadamide C6 (6)	<p>White powder MP: 185.7–188.3°C $[\alpha]_D^{20}$ +18.1° (<i>c</i> 0.006, MeOH) IR ($\nu_{\text{KB}}^{\text{cm}^{-1}}$): 3423, 1510, 1267, 1213, 1029 UV (MeOH) $\lambda_{\text{max}}(\log \epsilon)$: 280.6 nm ¹H NMR (600 MHz, CD₃OD): see Table VI. ¹³C NMR (150 MHz, CD₃OD): see Table VI. HMBC: see Figure 2. ESI-TOF-HR-MS: <i>m/z</i> 594.2054 [M+H]⁺; calcd. 594.2088 for C₃₀H₃₂N₃O₁₀ (2<i>R</i>,3<i>S</i>,2'<i>R</i>,3'<i>S</i>)-2-(3',4'-dihydroxyphenyl)-3-acetylamino-6-(3-acetylamino-6-(<i>N</i>-acetyl-2-amino-1-hydroxyethyl)-1,4-benzodioxan-2-yl)-1,4-benzodioxane</p>
Cicadamide C7 (7)	<p>White powder MP: 186.4–188.2°C $[\alpha]_D^{20}$ +12.9° (<i>c</i> 0.005, MeOH) IR ($\nu_{\text{KB}}^{\text{cm}^{-1}}$): 3466, 2314, 1269, 1028 UV (MeOH) $\lambda_{\text{max}}(\log \epsilon)$: 280.4 nm ¹H NMR (600 MHz, CD₃OD): see Table VII. ¹³C NMR (150 MHz, CD₃OD): see Table VII. HMBC: see Figure 2. ESI-TOF-HR-MS: <i>m/z</i> 594.2082 [M+H]⁺; calcd. 594.2088 for C₃₀H₃₂N₃O₁₀ (2<i>R</i>,3<i>S</i>,2'<i>R</i>,3'<i>S</i>)-2-(3',4'-dihydroxyphenyl)-3-acetylamino-6-(3-acetylamino-7-(<i>N</i>-acetyl-2-amino-1-hydroxyethyl)-1,4-benzodioxan-2-yl)-1,4-benzodioxane</p>

Table continued on next page.....

Compound	Detailed information
Cicadamide C8 (8)	<p>White powder MP: 186.6–187.4°C $[\alpha]_D^{20}$ +4.6° (<i>c</i> 0.002, MeOH) IR (ν_{KBr}, cm^{-1}): 3273, 3074, 1664, 1508, 1436, 1371, 1263, 1035 UV (MeOH) $\lambda_{\text{max}}(\log \epsilon)$: 280.8 nm ¹H NMR (600 MHz, CD₃OD): see Table VIII. ¹³C NMR (150 MHz, CD₃OD): see Table VIII. HMBC: see Figure 2. ESI-TOF-HR-MS: <i>m/z</i> 594.2012 [M+H]⁺; calcd. 594.2088 for C₃₀H₃₂N₃O₁₀ (2<i>R</i>,3<i>S</i>,2'<i>R</i>,3'<i>S</i>)-2-(3',4'-dihydroxyphenyl)-3-acetylamino-7-(3-acetylamino-7-(<i>N</i>-acetyl-2-amino-1-hydroxyethyl)-1,4-benzodioxan-2-yl)-1,4-benzodioxane</p>
Cicadamide C9 (9)	<p>White powder MP: 163.9–165.5°C IR (ν_{KBr}, cm^{-1}): 3269, 1649, 1508, 1271, 1033 UV (MeOH) $\lambda_{\text{max}}(\log \epsilon)$: 279.6 nm ¹H NMR (600 MHz, CD₃OD): see Table IX. ¹³C NMR (150 MHz, CD₃OD): see Table IX. HMBC: see Figure 2. ESI-TOF-HR-MS: <i>m/z</i> 576.1982 [M+H]⁺; calcd. 576.1982 for C₃₀H₃₀N₃O₉ (2<i>S</i>,3<i>R</i>,2'<i>R</i>,3'<i>S</i>)-2-(3',4'-dihydroxyphenyl)-3-acetylamino-7-(3-acetylamino-7-(<i>N</i>-acetyl-2-aminoethylene)-1,4-benzodioxan-2-yl)-1,4-benzodioxane</p>
Cicadamide C10 (10)	<p>White powder MP: 226.8–230.4°C $[\alpha]_D^{20}$ -26.3° (<i>c</i> -0.01, MeOH) IR (ν_{KBr}, cm^{-1}): 3275, 3061, 1649, 1502, 1437, 1373, 1269, 1020 UV (MeOH) $\lambda_{\text{max}}(\log \epsilon)$: 281.6 nm ¹H NMR (600 MHz, CD₃OD): see Table I0. ¹³C NMR (150 MHz, CD₃OD): see Table I0. HMBC: see Figure 2. ESI-TOF-HR-MS: <i>m/z</i> 576.1982 [M+H]⁺; calcd. 576.1982 for C₃₀H₃₀N₃O₉ (2<i>R</i>,3<i>S</i>,2'<i>R</i>,3'<i>S</i>)-2-(3',4'-dihydroxyphenyl)-3-acetylamino-7-(3-acetylamino-7-(<i>N</i>-acetyl-2-aminoethylene)-1,4-benzodioxan-2-yl)-1,4-benzodioxane</p>