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Crystal structure of (*E*)-resveratrol 3-*O*- β -*D*-xylopyranoside, C₁₉H₂₂O₈

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Abstract

C₁₉H₂₂O₈, orthorhombic, *P*2₁2₁2₁ (no. 19), *a* = 4.63150(10) Å, *b* = 9.4846(3) Å, *c* = 39.7929(11) Å, *V* = 1748.02(8) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0340, *wR*_{ref}(*F*²) = 0.0892, *T* = 150 K.

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The molecular structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.14 × 0.12 × 0.11 mm
Wavelength:	Cu Kα radiation (1.54184 Å)
μ:	0.95 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
θ _{max} , completeness:	67.4°, >99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	6494, 3156, 0.015
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 3118
<i>N</i> (<i>param</i>) _{refined} :	252
Programs:	CrysAlis ^{PRO} [1], Olex2 [2, 3], SHELX [4]

Source of material

The dry roots of *Lysidice rhodostegia* were purchased from Maoming, Guangdong Province, China. Dried Powder (14.0 kg) was extracted three times with 95% ethanol at room temperature. The solution was concentrated in vacuum to get a residue (1.5 kg). The crude extract was suspended in water and partitioned successively with petroleum ether, EtOAc and *n*-BuOH. The EtOAc extract (400.0 g) was chromatographed on a silica gel column eluted with CHCl₃–CH₃OH solvent system, afforded five fractions (Fr. 1–5). The title compound (systematic name: (*E*)-2-(3-hydroxy-5-(4-hydroxystyryl)phenoxy)tetrahydro-2H-pyran-3,4,5-triol) was obtained from Fr. 2 and crystallized in methanol.

Experimental details

A suitable crystal was selected and measured on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer. Using Olex2 [2], the structure was solved with the ShelXT [3]. Structure solution program using intrinsic phasing and the structure was refined with ShelXL [4].

Comment

The plant *L. rhodostegia* belongs to Leguminosae family. It is widely distributed in the south and southwest of China

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	X	Y	Z	U _{iso} [*] /U _{eq}
C1	0.6661 (4)	−0.10978 (18)	0.77330 (4)	0.0217 (4)
H1A	0.5372	−0.1843	0.7708	0.026*
C2	0.8223 (4)	−0.09742 (18)	0.80282 (4)	0.0229 (4)
H2A	0.8001	−0.1640	0.8198	0.027*
C3	1.0108 (4)	0.01379 (18)	0.80707 (4)	0.0191 (3)
C4	1.0466 (4)	0.11240 (18)	0.78147 (4)	0.0203 (3)
H4	1.1741	0.1872	0.7843	0.024*
C5	0.8922 (4)	0.09893 (18)	0.75181 (4)	0.0194 (3)
H5A	0.9181	0.1649	0.7348	0.023*
C6	0.6979 (4)	−0.01237 (17)	0.74702 (4)	0.0177 (3)
C7	0.5216 (4)	−0.03063 (18)	0.71664 (4)	0.0193 (3)
H7A	0.3860	−0.1029	0.7173	0.023*
C8	0.5327 (4)	0.04404 (17)	0.68826 (4)	0.0181 (3)
H8	0.6672	0.1166	0.6870	0.022*
C9	0.3462 (4)	0.01939 (17)	0.65882 (4)	0.0167 (3)
C10	0.1551 (4)	−0.09330 (17)	0.65721 (4)	0.0191 (3)
H10	0.1438	−0.1563	0.6751	0.023*
C11	−0.0181 (4)	−0.11252 (16)	0.62933 (4)	0.0177 (3)
C12	−0.0030 (4)	−0.02099 (16)	0.60223 (4)	0.0175 (3)
H12	−0.1181	−0.0346	0.5834	0.021*
C13	0.1871 (4)	0.09095 (16)	0.60392 (4)	0.0166 (3)
C14	0.3629 (4)	0.11371 (16)	0.63171 (4)	0.0171 (3)
H14	0.4891	0.1899	0.6323	0.020*
C15	0.3401 (4)	0.30353 (16)	0.57576 (4)	0.0153 (3)
H15	0.5437	0.2888	0.5815	0.018*
C16	0.3565 (4)	0.52341 (16)	0.60208 (4)	0.0188 (3)
H16A	0.5578	0.5053	0.6073	0.023*
H16B	0.2751	0.5791	0.6202	0.023*
C17	0.3340 (4)	0.60471 (16)	0.56908 (4)	0.0162 (3)
H17	0.1322	0.6307	0.5650	0.019*
C18	0.4434 (3)	0.51418 (16)	0.54018 (4)	0.0145 (3)
H18	0.6532	0.5044	0.5423	0.017*
C19	0.3088 (4)	0.36814 (16)	0.54100 (4)	0.0139 (3)
H19	0.1025	0.3773	0.5360	0.017*
O1	1.1597 (3)	0.02127 (13)	0.83677 (3)	0.0264 (3)
H1	1.2099	0.1029	0.8402	0.040*
O2	−0.2047 (3)	−0.22444 (12)	0.62964 (3)	0.0244 (3)
H2	−0.2956	−0.2263	0.6120	0.037*
O3	0.1890 (3)	0.17517 (11)	0.57499 (3)	0.0193 (3)
O4	0.2041 (3)	0.39266 (12)	0.59929 (3)	0.0190 (3)
O5	0.5038 (3)	0.72885 (11)	0.57221 (3)	0.0211 (3)
H5	0.4438	0.7890	0.5592	0.032*
O6	0.3804 (3)	0.58255 (13)	0.50906 (3)	0.0193 (3)
H6	0.5247	0.5822	0.4971	0.029*
O7	0.4367 (3)	0.27836 (12)	0.51610 (3)	0.0185 (3)
H7	0.5895	0.3129	0.5097	0.028*
O8	−0.1187 (3)	0.55432 (12)	0.47231 (3)	0.0205 (3)
H8A	0.0372	0.5486	0.4835	0.031*
H8B	−0.1393	0.4730	0.4637	0.031*

[5]. Previous chemical investigations of *L. rhodostegia* have revealed that phloroglucinol derivatives are the main chemical constituents of this plant [6, 7]. The roots of

this plant were proved to possess antioxidant [6], antiarrhythmia [8], and vasodilation [7] activities.

The title compound was determined structurally as (*E*)-resveratrol 3-*O*-β-D-xylopyranoside [7], which belongs to a class of stilbene derivatives. It has the basic skeleton of a stilbene combined with a D-xylose group. The C-O bond lengths 1.369(2)–1.4346(18) Å, C-C bond lengths of phenyl 1.381(2)–1.404(2) Å, C-C bond lengths of alkenyl 1.334(2) Å and the other C-C bond lengths 1.469(2)–1.526(2) Å, which were derived from the title structure are within normal ranges.

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