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# Malabaricone A isolated from a methanol extract of *Myristica malabarica*

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**Key indicators**

Single-crystal X-ray study
*T* = 299 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.046
*wR* factor = 0.143
Data-to-parameter ratio = 11.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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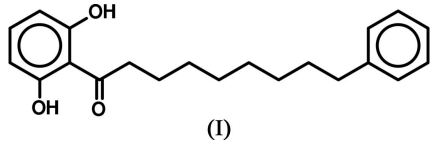
The title compound, malabaricone A [systematic name: 1-(2,6-dihydroxyphenyl)-9-phenylnonan-1-one], $C_{21}H_{26}O_3$, contains two benzene rings linked through a $C_9$ alkyl chain. Both intra- and intermolecular O—H···O hydrogen-bonding interactions stabilize the packing. The intermolecular hydrogen bonds result in the formation of an infinite zigzag chain.

## Comment

The fruit rind of *M. malabarica*, popularly known as Rampatri in Mumbai (India), is used as an exotic spice in various Indian cuisines, as well as in phytomedicine (Forrest & Heacock, 1972, and references therein). It is credited with hepatoprotective, anticarcinogenic and antithrombotic properties and is found as a constituent in many ayurvedic preparations such as Pasupasi.




(I)

Previous phytochemical investigations of *M. malabarica* fruit rinds revealed the presence of four novel diarylnonanoids, named as malabaricone A–D (Purushothaman *et al.*, 1977). In addition, a lignan malabericanol A and an isoflavone were also isolated from the heart wood of the plant (Purushathaman *et al.*, 1974; Talukdar *et al.*, 2000). During our studies on the antioxidant activity of methanol extracts of *M. malabarica* fruit rinds, we have isolated malabaricone A as a minor product. The compound was assayed against breast and colon cancer cells and the result found to be quite promising (Patro *et al.*, 2005).

The 2,6-dihydroxyphenyl and benzene rings are linked through a $C_9$ alkyl chain (Fig. 1). Intramolecular O—H···O hydrogen bonding results in the formation of a six-membered ring, while intermolecular O—H···O hydrgen bonding results in the formation of zigzag chains parallel to the *c* axis (Fig. 2). Details of the hydrogen bonding are given in Table 1.

## Experimental

The title compound was isolated as a minor product from a methanol extract of *M. malabarica* by column chromatography over silica gel with gradient elution by changing the polarity of the ethyl acetate–hexane solvent system. Crystals suitable for X-ray data collection were obtained by recrystallzation from hexane–benzene (4:1) at room temperature by evaporation.

*Crystal data*

$C_{21}H_{26}O_3$
$M_r$ = 326.47
Monoclinic, $P2_1/n$
$a$ = 4.1831 (6) Å
$b$ = 32.562 (2) Å
$c$ = 13.6270 (10) Å
$\beta$ = 98.430 (10)°
$V$ = 1836.1 (3) Å$^3$
$Z$ = 4
$D_x$ = 1.181 Mg m$^{-3}$
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta$ = 8.2–23.9°
$\mu$ = 0.61 mm$^{-1}$
$T$ = 299 (2) K
Prism, yellow
0.65 × 0.18 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
6403 measured reflections
3251 independent reflections
2092 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.044
$\theta_{max}$ = 67.1°
$h = -4 \rightarrow 4$
$k = -38 \rightarrow 0$
$l = -16 \rightarrow 16$
3 standard reflections
frequency: 120 min
intensity decay: 3.4%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.143
$S$ = 1.04
3251 reflections
296 parameters
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 0.1143P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0029 (5)

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1*O*···O3 | 0.92 (2) | 1.62 (2) | 2.4681 (19) | 151 (2) |
| O2—H2*O*···O1$^{i}$ | 0.88 (2) | 1.89 (2) | 2.7419 (18) | 164 (2) |

Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

The H atoms were located in a difference map and were refined with $U_{iso}$(H) = 1.2$U_{eq}$(parent atom).

Data collection: *CAD-4/PC Software* (Enraf–Nonius, 1993); cell refinement: *CAD-4/PC Software*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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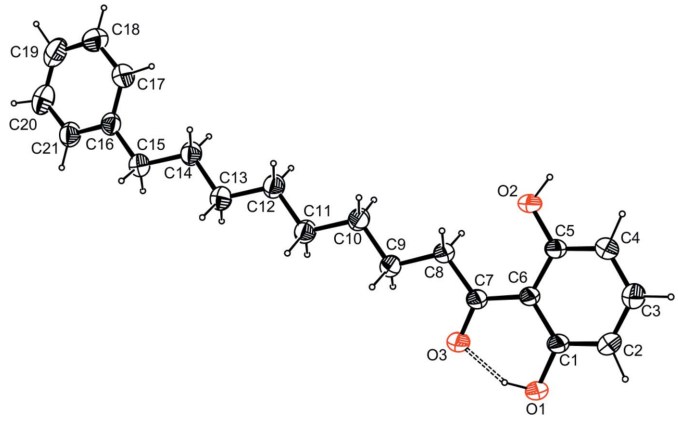


**Figure 1**
The molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probablity level. The dashed line indicates a hydrogen bond.

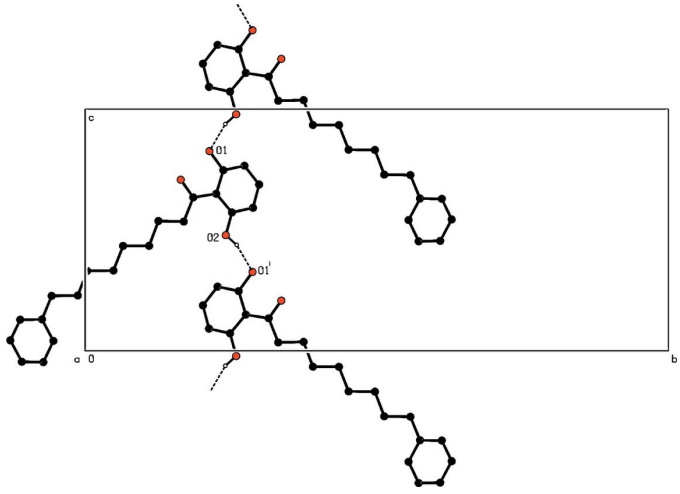


**Figure 2**
Part of the packing of the title compound showing the intermolecular O—H···O hydrogen bonds as dashed lines. [Symmetry code: (i) $x - \frac{1}{2}, \frac{1}{2} - y, z - \frac{1}{2}$.]

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