In the title compound, C_{21}H_{18}O_{4}, the relative conformation of the C=C and C=O double bonds in the central enone group is *s*-cisoid; there is a trans configuration about the C=C bond. The dihedral angle formed by the naphthalene ring system and the benzene ring is 16.80 (2)°. The methoxy groups at the ortho and para positions of the benzene ring are tilted to the ring by 169.8 (1)° and 174.5 (1)°, respectively. The hydroxy group in the benzene ring participates in an intramolecular O—H⋯O hydrogen bond. In the crystal, C—H⋯O interactions link molecules into linear chains along the a-axis direction.

Structure description

Reactive oxygen species (ROS) damage DNA, RNA, and proteins when present in excess. There is growing evidence that flavonoids can suppress carcinogenesis by inhibiting ROS levels (Rodríguez-García et al., 2019). Surprisingly, flavonoids can also induce excessive oxidative stress, leading to cancer cell death (Slika et al., 2022). Flavones (Hostetler et al., 2017), aurones (Sui et al., 2021), and chalcones (Elkanzi et al., 2022), which belong to the sub-group of flavonoids, have in common an α,β-unsaturated carbonyl group in the molecule. The α,β-unsaturated carbonyl group reacts with the thiol group of glutathione (GSH) as a Michael acceptor to reduce the intracellular GSH concentration (Adams et al., 2012). Since cancer cells have a higher ROS concentration than normal cells (Kumari et al., 2018), α,β-unsaturated carbonyl groups rapidly increase ROS levels due to decreased GSH, thereby killing cancer cells (Raj et al., 2011). As an extension of the search for ROS-generating compounds in cancer cells (Shin et al., 2022; Lee et al., 2016), the title chalcone compound was synthesized.

The molecular structure of the title compound is shown in Fig. 1. In the central α,β-unsaturated carbonyl group, the carbonyl O1⋯C1 and C2⋯C3 double bonds are twisted at an angle of −22.9 (2)° for the C3—C2—C1—O1 torsion angle. A trans-configuration is
noted for the C2=C3 double bond, which has a torsion angle of $-178.3(1)^\circ$ for C1–C2–C3–C4. The methoxy group at the para position (C-17) of the benzene ring is nearly coplanar with the ring [C18–C17–O3–C20 $= 174.5(1)^\circ$], while the other methoxy group at the ortho position (C-19) is more twisted out of the ring [C14–C19–O4–C21 $= 169.8(1)^\circ$].

The naphthalene ring system (C4–C13; r.m.s. deviation of 0.003 Å) is tilted at an angle of 16.80 (2)$^\circ$ with respect to the benzene ring (C14–C19; r.m.s. deviation of 0.011 Å). The hydroxy group attached to the benzene ring is involved in an intramolecular O–H···O hydrogen bond. In the crystal, weak C–H···O interactions link the molecules into linear chains propagating along the $a$-axis direction (Fig. 2).

**Synthesis and crystallization**

1-(2-Hydroxy-4,6-dimethoxyphenyl)ethanone (196 mg, 1 mmol) and 1-naphthaldehyde (156 mg, 1 mmol) were dissolved in ethanol (25 ml) and the temperature was cooled to around 276–277 K in an ice bath. To the cooled reaction mixture were added 1.0 ml of 40% aqueous KOH solution, and the reaction mixture was stirred at room temperature for 20 h. This mixture was poured into iced water (40 ml) and acidified with 6 N HCl solution. The mixture was extracted with ethyl acetate (2 × 30 ml) and the combined organic layers were dried over MgSO4. Filtration and evaporation of the filtrate gave a residue which was purified by flash chromatography to give the title compound (260 mg, 78%). Recrystallization in ethanol gave the crystals used in this X-ray diffraction study.

**Refinement**

Crystal data, data collection and structure refinement details are summarized in Table 2.

**Acknowledgements**

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full crystallographic data

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(E)-1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-(naphthalen-1-yl)prop-2-en-1-one

Dongsoo Koh

(E)-1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-(naphthalen-1-yl)prop-2-en-1-one

Crystal data

C₂₁H₁₈O₄  \( \cdot \)
\( M_r = 334.35 \)
Monoclinic, \( C2/c \)
Hall symbol: \(-C 2yc\)
\( a = 15.8594 \) Å
\( b = 5.0437 \) Å
\( c = 40.6908 \) Å
\( \beta = 90.507 \)°
\( V = 3254.7 \) Å³
\( Z = 8 \)

\( F(000) = 1408 \)
\( D_x = 1.365 \) Mg m⁻³
\( Cu \) \( K\alpha \) radiation, \( \lambda = 1.54178 \) Å

Cell parameters from 6156 reflections
\( \theta = 6.5–66.5° \)
\( \mu = 0.77 \) mm⁻¹
\( T = 147 \) K
Needle, yellow

0.65 × 0.11 × 0.03 mm

Data collection

Bruker Kappa APEX DUO CCD diffractometer
Radiation source: Bruker ImuS Multi-layer optics monochromator
\( \phi \) and \( \omega \) scans
Absorption correction: multi-scan
(SADABS; Bruker, 2012)
\( T_{\text{min}} = 0.655, T_{\text{max}} = 0.753 \)

10590 measured reflections
2743 independent reflections
2555 reflections with \( I > 2 \sigma(I) \)

\( R_{\text{int}} = 0.027 \)
\( \theta_{\text{max}} = 66.5°, \theta_{\text{min}} = 6.5° \)
\( h = -18→18 \)
\( k = -5→1 \)
\( l = -48→47 \)

Refinement

Refinement on \( F^2 \)
Least-squares matrix: full
\( R[F^2 > 2\sigma(F^2)] = 0.037 \)
\( wR(F^2) = 0.098 \)
\( S = 1.03 \)
2743 reflections
232 parameters
0 restraints

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
\( w = 1[\sigma(F_c^2) + (0.0514P)^2 + 2.058P] \)
where \( P = (F_c^2 + 2F_s^2)/3 \)

\( (\Delta/\sigma)_{\text{max}} = 0.001 \)
\( \Delta \rho_{\text{max}} = 0.16 \) e Å⁻³
\( \Delta \rho_{\text{min}} = -0.22 \) e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.
**Refinement.** Refinement of F² against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F², conventional R-factors R are based on F, with F set to zero for negative F². The threshold expression of F² > 2σ(F²) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F² are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

| Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²) | x      | y      | z      | Uiso*/Ueq |
|-----------------------------------------------|--------|--------|--------|-----------|
| O1    | 0.83835 (5) | 0.92735 (19) | 0.40390 (2) | 0.0331 (2) |
| O2    | 0.82944 (5) | 1.26680 (18) | 0.44807 (2) | 0.0286 (2) |
| O3    | 0.56231 (5) | 1.62372 (18) | 0.47470 (2) | 0.0289 (2) |
| O4    | 0.57849 (5) | 0.93109 (17) | 0.39751 (2) | 0.0277 (2) |
| C1    | 0.75984 (8) | 0.9014 (2)   | 0.40286 (3) | 0.0233 (3) |
| C2    | 0.72497 (8) | 0.6836 (3)   | 0.38301 (3) | 0.0278 (3) |
| H2A   | 0.6702     | 0.6195     | 0.3880   | 0.033*    |
| C3    | 0.76623 (8) | 0.5731 (2)   | 0.35859 (3) | 0.0267 (3) |
| H3A   | 0.8215     | 0.6365     | 0.3543   | 0.032*    |
| C4    | 0.73370 (8) | 0.3599 (2)   | 0.33742 (3) | 0.0239 (3) |
| C5    | 0.64822 (8) | 0.3106 (3)   | 0.33554 (3) | 0.0284 (3) |
| H5A   | 0.6109     | 0.4154     | 0.3483   | 0.034*    |
| C6    | 0.61469 (9) | 0.1099 (3)   | 0.31536 (3) | 0.0309 (3) |
| H6A   | 0.5555     | 0.0802     | 0.3147   | 0.037*    |
| C7    | 0.66664 (9) | −0.0425 (3) | 0.29668 (3) | 0.0294 (3) |
| H7A   | 0.6435     | −0.1779    | 0.2831   | 0.035*    |
| C8    | 0.75456 (8) | −0.0002 (2) | 0.29737 (3) | 0.0250 (3) |
| C9    | 0.80929 (9) | −0.1570 (3) | 0.27802 (3) | 0.0319 (3) |
| H9A   | 0.7863     | −0.2930    | 0.2645   | 0.038**   |
| C10   | 0.89410 (10) | −0.1162 (3) | 0.27848 (3) | 0.0371 (3) |
| H10A  | 0.9298     | −0.2226    | 0.2653   | 0.045*    |
| C11   | 0.92890 (9) | 0.0833 (3)   | 0.29851 (4) | 0.0363 (3) |
| H11A  | 0.9882     | 0.1111     | 0.2988   | 0.044*    |
| C12   | 0.87801 (8) | 0.2379 (3)   | 0.31759 (3) | 0.0294 (3) |
| H12A  | 0.9026     | 0.3716     | 0.3310   | 0.035*    |
| C13   | 0.78924 (8) | 0.2026 (2)   | 0.31770 (3) | 0.0232 (3) |
| C14   | 0.70640 (8) | 1.0824 (2)   | 0.42166 (3) | 0.0212 (3) |
| C15   | 0.74516 (7) | 1.2624 (2)   | 0.44389 (3) | 0.0220 (3) |
| C16   | 0.69958 (8) | 1.4415 (2)   | 0.46266 (3) | 0.0230 (3) |
| H16A  | 0.7273     | 1.5536     | 0.4781   | 0.028**   |
| C17   | 0.61307 (8) | 1.4532 (2)   | 0.45848 (3) | 0.0232 (3) |
| C18   | 0.57152 (8) | 1.2849 (2)   | 0.43638 (3) | 0.0240 (3) |
| H18A  | 0.5121     | 1.2976     | 0.4335   | 0.029**   |
| C19   | 0.61656 (8) | 1.1008 (2)   | 0.41876 (3) | 0.0216 (3) |
| C20   | 0.60019 (9) | 1.7843 (3)   | 0.49980 (3) | 0.0298 (3) |
| H20A  | 0.5563     | 1.8845     | 0.5112   | 0.045*    |
| H20B  | 0.6402     | 1.9079     | 0.4898   | 0.045*    |
| H20C  | 0.6300     | 1.6705     | 0.5156   | 0.045*    |
| C21   | 0.48877 (9) | 0.9150 (3)   | 0.39821 (4) | 0.0405 (4) |
|      |         |         |         |         |         |         |
|------|---------|---------|---------|---------|---------|---------|
| H21A | 0.4699  | 0.7638  | 0.3849  | 0.061*  |
| H21B | 0.4645  | 1.0787  | 0.3893  | 0.061*  |
| H21C | 0.4703  | 0.8914  | 0.4209  | 0.061*  |
| H2O  | 0.8485 (12) | 1.142 (4) | 0.4325 (5) | 0.064 (6)* |

**Atomic displacement parameters (Å²)**

|      | U₁¹₁ | U₂²₂ | U₃₃₃ | U₁₂₂ | U₁₃₃ | U₂₃₃ |
|------|------|------|------|------|------|------|
| O1   | 0.0226 (5) | 0.0357 (5) | 0.0409 (5) | 0.0010 (4) | 0.0022 (4) | −0.0128 (4) |
| O2   | 0.0200 (5) | 0.0321 (5) | 0.0336 (5) | −0.0005 (4) | −0.0009 (4) | −0.0081 (4) |
| O3   | 0.0249 (5) | 0.0318 (5) | 0.0300 (5) | 0.0043 (4) | 0.0027 (4) | −0.0074 (4) |
| O4   | 0.0236 (5) | 0.0297 (5) | 0.0297 (5) | −0.0045 (4) | −0.0016 (4) | −0.0066 (4) |
| C1   | 0.0257 (6) | 0.0215 (6) | 0.0226 (6) | −0.0003 (5) | 0.0024 (5) | 0.0037 (5) |
| C2   | 0.0258 (7) | 0.0260 (7) | 0.0318 (7) | −0.0011 (5) | 0.0024 (5) | −0.0035 (5) |
| C3   | 0.0247 (6) | 0.0260 (7) | 0.0294 (6) | 0.0011 (5) | −0.0008 (5) | −0.0029 (5) |
| C4   | 0.0280 (7) | 0.0229 (6) | 0.0208 (6) | 0.0006 (5) | −0.0006 (5) | 0.0020 (5) |
| C5   | 0.0289 (7) | 0.0280 (7) | 0.0283 (6) | 0.0008 (5) | 0.0018 (5) | −0.0009 (5) |
| C6   | 0.0278 (7) | 0.0334 (7) | 0.0313 (7) | −0.0060 (6) | −0.0026 (5) | 0.0016 (6) |
| C7   | 0.0385 (8) | 0.0259 (7) | 0.0238 (6) | −0.0061 (6) | −0.0059 (5) | 0.0001 (5) |
| C8   | 0.0352 (7) | 0.0216 (6) | 0.0182 (6) | 0.0002 (5) | −0.0021 (5) | 0.0035 (5) |
| C9   | 0.0446 (8) | 0.0268 (7) | 0.0243 (6) | 0.0008 (6) | −0.0007 (6) | −0.0043 (5) |
| C10  | 0.0420 (8) | 0.0352 (8) | 0.0342 (7) | 0.0078 (6) | 0.0074 (6) | −0.0073 (6) |
| C11  | 0.0303 (7) | 0.0374 (8) | 0.0414 (8) | 0.0035 (6) | 0.0042 (6) | −0.0048 (6) |
| C12  | 0.0298 (7) | 0.0275 (7) | 0.0310 (7) | 0.0000 (5) | −0.0001 (5) | −0.0041 (5) |
| C13  | 0.0293 (7) | 0.0209 (6) | 0.0194 (6) | 0.0013 (5) | −0.0011 (5) | 0.0030 (5) |
| C14  | 0.0236 (6) | 0.0195 (6) | 0.0206 (6) | −0.0016 (5) | 0.0017 (5) | 0.0024 (5) |
| C15  | 0.0215 (6) | 0.0224 (6) | 0.0219 (6) | −0.0017 (5) | 0.0004 (5) | 0.0040 (5) |
| C16  | 0.0257 (6) | 0.0225 (6) | 0.0208 (6) | −0.0020 (5) | 0.0002 (5) | −0.0015 (5) |
| C17  | 0.0261 (6) | 0.0220 (6) | 0.0217 (6) | 0.0018 (5) | 0.0044 (5) | 0.0019 (5) |
| C18  | 0.0200 (6) | 0.0264 (7) | 0.0257 (6) | −0.0005 (5) | 0.0007 (5) | 0.0020 (5) |
| C19  | 0.0243 (6) | 0.0210 (6) | 0.0195 (6) | −0.0037 (5) | 0.0003 (5) | 0.0026 (5) |
| C20  | 0.0331 (7) | 0.0314 (7) | 0.0249 (6) | 0.0060 (6) | 0.0009 (5) | −0.0055 (5) |
| C21  | 0.0231 (7) | 0.0492 (9) | 0.0490 (9) | −0.0054 (6) | −0.0050 (6) | −0.0144 (7) |

**Geometric parameters (Å, °)**

|      |         |         |         |         |         |         |
|------|---------|---------|---------|---------|---------|---------|
| O1—C1 | 1.2523 (15) |         |         |         |         |         |
| O2—C15 | 1.3461 (15) |         |         |         |         |         |
| O2—H2O | 0.94 (2) |         |         |         |         |         |
| O3—C17 | 1.3538 (15) |         |         |         |         |         |
| O3—C20 | 1.4316 (15) |         |         |         |         |         |
| O4—C19 | 1.3549 (15) |         |         |         |         |         |
| O4—C21 | 1.4258 (16) |         |         |         |         |         |
| C1—C14 | 1.4656 (17) |         |         |         |         |         |
| C1—C2 | 1.3823 (17) |         |         |         |         |         |
| C2—C3 | 1.3182 (19) |         |         |         |         |         |
| C2—H2A | 0.9500 |         |         |         |         |         |

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| Bond                  | Distance (Å) | Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|----------------------|-------------|----------------------|-------------|----------------------|-------------|
| C3—H3A               | 0.9500      | C16—H16A             | 0.9500      | C17—C18              | 1.3974 (18) |
| C4—C5                | 1.3797 (18) | C17—H18A             | 0.9500      | C20—H20A             | 0.9800      |
| C4—C13               | 1.4360 (17) | C18—C19              | 1.3769 (17) | C20—H20B             | 0.9800      |
| C5—C6                | 1.4051 (19) | C18—H18A             | 0.9500      | C20—H20C             | 0.9800      |
| C6—C7                | 1.363 (2)   | C20—H21A             | 0.9800      | C21—H21B             | 0.9800      |
| C6—H6A               | 0.9500      | C20—H21A             | 0.9800      | C21—H21C             | 0.9800      |
| C7—C8                | 1.4105 (19) | C21—H21B             | 0.9800      |
| C7—H7A               | 0.9500      | C21—H21C             | 0.9800      |
| C8—C9                | 1.4178 (18) |                      |             |                      |             |
| C8—C13               | 1.4232 (18) |                      |             |                      |             |
| C15—O2—H2O           | 103.2 (12)  | C11—C12—C13          | 121.35 (12) |
| C17—O3—C20           | 117.37 (10) | C11—C12—H12A         | 119.3       |
| C19—O4—C21           | 117.53 (10) | C13—C12—H12A         | 119.3       |
| O1—C1—C14            | 119.78 (11) | C12—C13—C8           | 117.82 (11) |
| O1—C1—C2             | 117.78 (11) | C12—C13—C4           | 123.08 (11) |
| C14—C1—C2            | 122.42 (11) | C8—C13—C4            | 119.09 (11) |
| C3—C2—C1             | 122.95 (12) | C15—C14—C19          | 115.88 (11) |
| C3—C2—H2A            | 118.5       | C15—C14—C1           | 118.83 (11) |
| C1—C2—H2A            | 118.5       | C19—C14—C1           | 125.25 (11) |
| C2—C3—C4             | 125.29 (12) | O2—C15—C16           | 116.16 (11) |
| C2—C3—H3A            | 117.4       | O2—C15—C14           | 121.02 (11) |
| C4—C3—H3A            | 117.4       | C16—C15—C14          | 122.82 (11) |
| C5—C4—C13            | 118.47 (11) | C17—C16—C15          | 118.74 (11) |
| C5—C4—C3             | 120.29 (11) | C17—C16—H16A         | 120.6       |
| C13—C4—C3            | 121.22 (11) | C15—C16—H16A         | 120.6       |
| C4—C5—C6             | 121.93 (12) | O3—C17—C16           | 124.13 (11) |
| C4—C5—H5A            | 119.0       | O3—C17—C18           | 114.87 (11) |
| C6—C5—H5A            | 119.0       | C16—C17—C18          | 121.00 (11) |
| C7—C6—C5             | 120.30 (12) | C19—C18—C17          | 120.06 (11) |
| C7—C6—H6A            | 119.8       | C19—C18—H18A         | 120.0       |
| C5—C6—H6A            | 119.8       | C17—C18—H18A         | 120.0       |
| C6—C7—C8             | 120.41 (12) | O4—C19—C18           | 121.88 (11) |
| C6—C7—H7A            | 119.8       | O4—C19—C14           | 116.69 (10) |
| C8—C7—H7A            | 119.8       | C18—C19—C14          | 121.43 (11) |
| C7—C8—C9             | 120.98 (12) | O3—C20—H20A          | 109.5       |
| C7—C8—C13            | 119.80 (11) | O3—C20—H20B          | 109.5       |
| C9—C8—C13            | 119.22 (12) | H20A—C20—H20B        | 109.5       |
| C10—C9—C8            | 121.20 (12) | O3—C20—H20C          | 109.5       |
| C10—C9—H9A           | 119.4       | H20A—C20—H20C        | 109.5       |
| C8—C9—H9A            | 119.4       | H20B—C20—H20C        | 109.5       |
| C9—C10—C11           | 119.97 (13) | O4—C21—H21A          | 109.5       |
| C9—C10—H10A          | 120.0       | O4—C21—H21B          | 109.5       |
| C11—C10—H10A         | 120.0       | H21A—C21—H21B        | 109.5       |
| C12—C11—C10          | 120.43 (13) | O4—C21—H21C          | 109.5       |
| C12—C11—H11A         | 119.8       | H21A—C21—H21C        | 109.5       |
| C10—C11—H11A         | 119.8       | H21B—C21—H21C        | 109.5       |
O1—C1—C2—C3  -22.91 (19)  C3—C4—C13—C8  -179.47 (11)
C14—C1—C2—C3  158.34 (12)  O1—C1—C14—C15  -7.79 (17)
C1—C2—C3—C4  -178.35 (11)  C2—C1—C14—C15  169.92 (11)
C2—C3—C4—C5  -162.71 (13)  C2—C1—C14—C19  -11.36 (18)
C13—C4—C5—C6  0.90 (18)  C1—C14—C15—O2  -0.65 (16)
C3—C4—C5—C6  179.46 (12)  C19—C14—C15—O2  1.93 (17)
C4—C5—C6—C7  -0.4 (2)  C19—C14—C15—C16  179.84 (11)
C5—C6—C7—C8  -0.08 (19)  C2—C1—C14—C19  170.93 (11)
C6—C7—C8—C9  -179.90 (12)  C2—C3—C4—C13  -162.71 (13)
C6—C7—C8—C13  0.03 (18)  C13—C4—C5—C6  179.46 (12)
C7—C8—C9—C10  179.69 (12)  C3—C4—C5—C6  18.8 (2)
C13—C8—C9—C10  -0.25 (19)  C4—C5—C6—C7  -0.4 (2)
C8—C9—C10—C11  0.3 (2)  C5—C6—C7—C8  -0.08 (19)
C9—C10—C11—C12  -0.1 (2)  C6—C7—C8—C13  0.03 (18)
C10—C11—C12—C13  -0.2 (2)  C7—C8—C9—C10  -0.25 (19)
C11—C12—C13—C8  0.25 (19)  C8—C9—C10—C11  0.3 (2)
C11—C12—C13—C4  179.78 (12)  C9—C10—C11—C12  -0.1 (2)
C7—C8—C13—C12  -179.98 (11)  C10—C11—C12—C13  -0.2 (2)
C9—C8—C13—C12  -0.05 (17)  C11—C12—C13—C4  0.25 (19)
C7—C8—C13—C4  0.46 (17)  C8—C9—C10—C11  -0.1 (2)
C9—C8—C13—C4  -179.60 (11)  C11—C12—C13—C8  0.25 (19)
C5—C4—C13—C12  179.56 (11)  C9—C8—C13—C4  -179.60 (11)
C3—C4—C13—C12  1.01 (18)  C5—C4—C13—C8  -0.91 (17)
C5—C4—C13—C8  -177.10 (11)  O2—O···O  0.94 (2)  1.60 (2)  2.4869 (12)  155.5 (18)

Symmetry code: (i) x−1/2, y−1/2, z.