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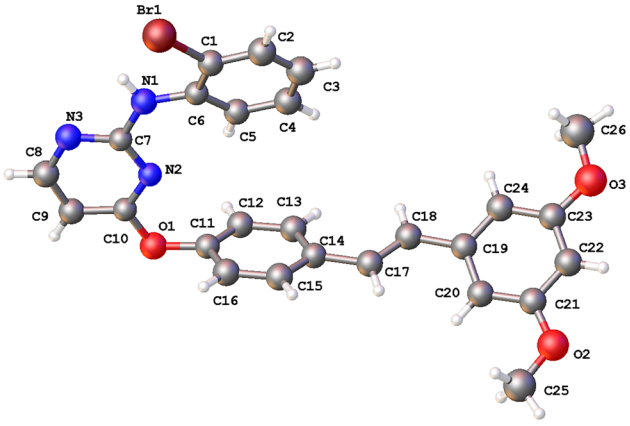
# Crystal structure of (*E*)-*N*-(2-bromophenyl)-4-(4-(3,5-dimethoxystyryl)phenoxy)pyrimidin-2-amine, $C_{26}H_{22}BrN_3O_3$




https://doi.org/10.1515/ncrs-2024-0187
Received April 27, 2024; accepted May 30, 2024;
published online June 20, 2024

**Abstract**

$C_{26}H_{22}BrN_3O_3$, monoclinic, $P2_1/c$ (no. 14), $a$ = 17.7467(15) Å, $b$ = 10.7974(8) Å, $c$ = 11.9136(8) Å, $\beta$ = 96.084°, $V$ = 2270.0(3) Å$^3$, $Z$ = 4, $R_{gt}(F)$ = 0.0375, $wR_{ref}(F^2)$ = 0.1205, T = 293 K.

**CCDC no.:** 2350232

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.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Colourless block |
| Size: | 0.25 × 0.23 × 0.20 mm |
| Wavelength: | Mo *K*α radiation (0.71073 Å) |
| $\mu$: | 1.85 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 25.0°, >99 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 26,554, 3,990, 0.052 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\sigma(I_{obs})$, 3,133 |
| $N(param)_{refined}$: | 300 |
| Programs: | Bruker,[1] SHELX[2,3] |

## 1 Source of material

Pterostilbene (256 mg, 1 mmol) and 1,4-dioxane (20 mL) were added in a solution of sodium hydroxide (40 mg, 1 mmol) in water (10 mL) and the mixture was maintained at ice-bath temperature. To this was added, dropwise, a solution of 2,4-dichloroprymidine (149 mg, 1 mmol) in 1,4-dioxane (20 mL). The reaction was monitored by thin layer chromatography (TLC, petroleum ether:ethyl acetate = 4:1, *v*/*v*). When the reaction was completed, the mixture was concentrated under vacuum and recrystallized from ethyl acetate. The intermediate (*E*)-2-chloro-4-(4-(3,5-dimethoxystyryl)phenoxy)pyrimidine was obtained as a white soild. The intermediate (368 mg, 1 mmol) and 2-bromoaniline (172 mg, 1 mmol) were dissolved in isopropyl alcohol (10 mL), and concentrated hydrochloric acid (2–3 drops) was added. The reaction mixture was reacted at reflux temperature for 4 h. After the reaction was finished, the mixture was concentrated under reduced pressure and extracted with ethyl acetate (30 mL). The organic layer was washed with brine (25 mL × 3), dried, filtered and concentrated. The residue was purified by recrystallization (ethyl acetate). The crystals of the title compound were grown by slow evaporation of its dichloromethane:n-hexane (1:2, *v*/*v*) solution at room temperature.

## 2 Experimental details

All hydrogen atoms were placed in the calculated positions and all the non-hydrogen atoms were refined anisotropically.

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**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| Atom | x | y | z | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.88233 (2) | −0.02634 (3) | 0.99632 (3) | 0.08232 (18) |
| C1 | 0.84729 (13) | 0.0981 (2) | 0.89158 (19) | 0.0480 (5) |
| C2 | 0.80088 (15) | 0.0615 (3) | 0.7965 (2) | 0.0569 (6) |
| H2 | 0.788148 | −0.021486 | 0.785856 | 0.068* |
| C3 | 0.77382 (14) | 0.1479 (3) | 0.7184 (2) | 0.0585 (7) |
| H3 | 0.742727 | 0.123915 | 0.654327 | 0.070* |
| C4 | 0.79299 (14) | 0.2710 (3) | 0.7353 (2) | 0.0533 (6) |
| H4 | 0.773879 | 0.329921 | 0.682881 | 0.064* |
| C5 | 0.84016 (13) | 0.3074 (2) | 0.82895 (19) | 0.0474 (5) |
| H5 | 0.853412 | 0.390472 | 0.837892 | 0.057* |
| C6 | 0.86833 (12) | 0.2216 (2) | 0.91054 (17) | 0.0406 (5) |
| C7 | 0.92939 (12) | 0.3623 (2) | 1.06037 (17) | 0.0395 (5) |
| C8 | 0.99197 (14) | 0.4675 (2) | 1.2043 (2) | 0.0509 (6) |
| H8 | 1.025998 | 0.469589 | 1.269212 | 0.061* |
| C9 | 0.95853 (13) | 0.5762 (2) | 1.16860 (18) | 0.0481 (6) |
| H9 | 0.969378 | 0.651087 | 1.205361 | 0.058* |
| C10 | 0.90707 (12) | 0.5661 (2) | 1.07316 (17) | 0.0400 (5) |
| C11 | 0.81285 (13) | 0.6552 (2) | 0.94275 (18) | 0.0437 (5) |
| C12 | 0.82842 (14) | 0.6845 (2) | 0.8353 (2) | 0.0498 (6) |
| H12 | 0.877187 | 0.707039 | 0.821681 | 0.060* |
| C13 | 0.77079 (14) | 0.6800 (2) | 0.7480 (2) | 0.0495 (6) |
| H13 | 0.781488 | 0.698303 | 0.675054 | 0.059* |
| C14 | 0.69701 (13) | 0.6487 (2) | 0.76656 (19) | 0.0448 (5) |
| C15 | 0.68371 (14) | 0.6195 (2) | 0.8763 (2) | 0.0521 (6) |
| H15 | 0.635029 | 0.597460 | 0.890928 | 0.063* |
| C16 | 0.74112 (14) | 0.6223 (2) | 0.9645 (2) | 0.0522 (6) |
| H16 | 0.731238 | 0.602169 | 1.037369 | 0.063* |
| C17 | 0.63315 (14) | 0.6485 (2) | 0.6779 (2) | 0.0495 (6) |
| H17 | 0.585181 | 0.653871 | 0.702264 | 0.059* |
| C18 | 0.63530 (14) | 0.6417 (2) | 0.5672 (2) | 0.0503 (6) |
| H18 | 0.682696 | 0.636365 | 0.540920 | 0.060* |
| C19 | 0.56841 (14) | 0.6418 (2) | 0.48257 (19) | 0.0493 (6) |
| C20 | 0.49824 (14) | 0.6819 (2) | 0.50969 (18) | 0.0506 (6) |
| H20 | 0.493203 | 0.712757 | 0.581390 | 0.061* |
| C21 | 0.43554 (15) | 0.6758 (2) | 0.4293 (2) | 0.0517 (6) |
| C22 | 0.44241 (15) | 0.6316 (3) | 0.3228 (2) | 0.0541 (6) |
| H22 | 0.400093 | 0.627162 | 0.269814 | 0.065* |
| C23 | 0.51149 (15) | 0.5943 (2) | 0.29503 (19) | 0.0518 (6) |
| C24 | 0.57548 (14) | 0.5988 (2) | 0.3740 (2) | 0.0531 (6) |
| H24 | 0.622375 | 0.573392 | 0.354193 | 0.064* |
| C25 | 0.35050 (17) | 0.7496 (4) | 0.5553 (2) | 0.0760 (9) |
| H25A | 0.363408 | 0.684629 | 0.608923 | 0.114* |
| H25B | 0.297893 | 0.770332 | 0.555396 | 0.114* |
| H25C | 0.380933 | 0.821308 | 0.575679 | 0.114* |
| C26 | 0.5809 (2) | 0.5067 (3) | 0.1525 (3) | 0.0817 (9) |
| H26A | 0.618187 | 0.571345 | 0.161651 | 0.123* |
| H26B | 0.573217 | 0.482536 | 0.074552 | 0.123* |
| H26C | 0.598196 | 0.436667 | 0.197735 | 0.123* |
| N1 | 0.91724 (12) | 0.25094 (18) | 1.00624 (15) | 0.0496 (5) |
| H1 | 0.943712 | 0.190136 | 1.035664 | 0.059* |
| N2 | 0.89218 (10) | 0.46201 (17) | 1.01814 (15) | 0.0398 (4) |
| N3 | 0.97961 (11) | 0.35833 (19) | 1.15302 (16) | 0.0493 (5) |
| O1 | 0.86971 (9) | 0.66936 (15) | 1.03381 (14) | 0.0529 (4) |
| O2 | 0.36393 (10) | 0.7099 (2) | 0.44802 (15) | 0.0708 (6) |
| O3 | 0.51207 (13) | 0.5501 (2) | 0.18695 (16) | 0.0735 (6) |

# 3 Comment

Pterostilbene, chemically related to resveratrol, is not only an active phytonutrient but also a potential drug with multiple biomedical applications.[4–8] In this paper, we report the synthesis and crystal structure of a novel pterostilbene compound with a pyrimidine fragment. Single-crystal structure analysis reveals that there is one molecule in the asymmetric unit (*cf.* figure). Its molecular structure contains a pyrimidine ring, three benzene rings, a carbon–carbon double bond and two methoxy groups. The pyrimidine ring and two benzene rings are linked by N(1) atom and O(1) atom. The two benzene rings are linked by the carbon–carbon double bond. The carbon-carbon double bond and the attached benzene rings are also approximately coplanar, while the dihedral angle of the two benzene rings is 37.93°. The two methoxy groups (C21–O2–C25 and C23–O3–C26) are in the same plane as their attached benzene ring and their dihedral angles to the attached benzene ring are 3.09 and 1.21°, respectively. The torsion angles of C6–N1–C7 and C10–O1–C11 are 129.56 and 117.45°. All bond angles and lengths are within the normal range.[9] And the structural characteristics of the title compound are similar to those of *N*-phenyl-4-(4-(2-(2-pyridinyl) ethenyl)phenoxy)picolinamide[10] and (*E*)-4-(6-(4-(2-(pyridin-4-yl)vinyl)phenoxy)pyrimidin-4-yl)morpholine.[11]

The complete set of X-ray diffraction data for the title compound was deposited to the Cambridge Crystallographic Data Centre (CCDC entry no. 2350232).

**Author contribution**: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.
**Conflict of interest statement**: The authors declare no conflicts of interest regarding this article.
**Research funding**: None declared.

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