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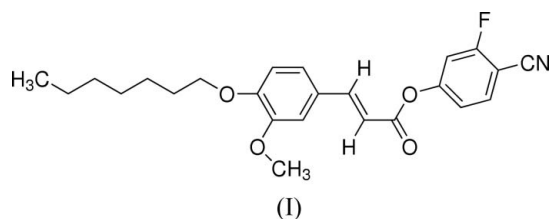
## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
Disorder in main residue  
 $R$  factor = 0.057  
 $wR$  factor = 0.160  
Data-to-parameter ratio = 14.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.4-Cyano-3-fluorophenyl (2*E*)-3-(4-heptyloxy-3-methoxyphenyl)acrylate

In the title compound,  $\text{C}_{24}\text{H}_{26}\text{FNO}_4$ , the two benzene rings are almost perpendicular to one another, with a dihedral angle of  $87.7(1)^\circ$ . Molecules are linked into two-dimensional layers by non-classical intermolecular hydrogen-bonding interactions. The packing is further stabilized by  $\pi$ - $\pi$  interactions.

## Comment

We have reported the structure of 4-cyano-3-fluorophenyl 4'-isobutoxybiphenyl-4-carboxylate, (II) (Ren *et al.*, 2005). In our ongoing research into liquid-crystal materials containing fluorine, the title compound, (I), was obtained and its structure is reported here.



Bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987), and the values in the 4-cyano-3-fluorophenyl group are comparable with those in the related structure 4-cyano-3-fluorophenyl 4'-isobutoxybiphenyl-4-carboxylate (Ren *et al.*, 2005). The 4-heptyloxy-3-methoxyphenyl group, excluding atom C24, is essentially coplanar with the acrylate fragment. This combined unit is almost perpendicular to the 4-cyano-3-fluorophenyl group, with a dihedral angle of  $87.7(1)^\circ$  between the two benzene rings. The C8—C9—C10—C11 torsion angle is  $178.9(2)^\circ$ , indicating a *trans* configuration of the double bond. The F atom shows disorder over two positions, with site occupancies of 0.638 (4) and 0.362 (4).

There is one intramolecular hydrogen-bond interaction, C10—H10 $\cdots$ O1, forming a five-membered ring, which contributes to the planarity of the acrylate group. In the crystal structure, molecules are linked into two-dimensional

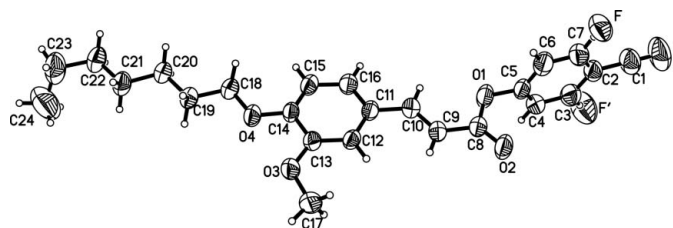
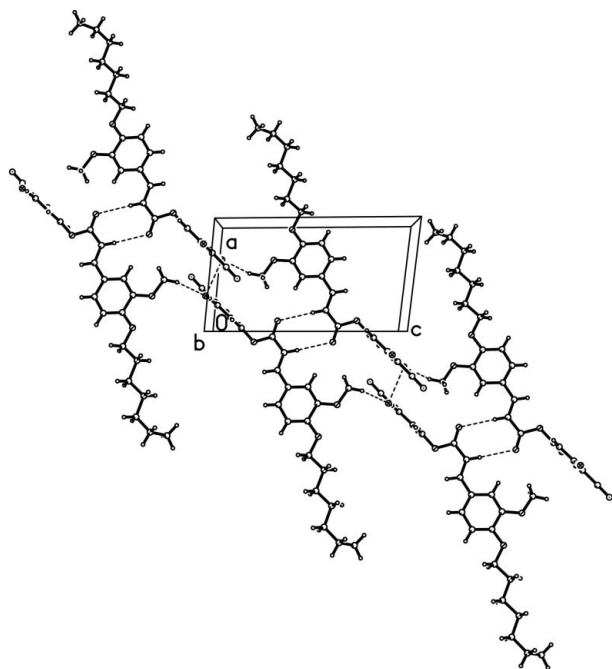


Figure 1

The structure of the compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The fluorine is disordered over two positions. Both components are shown.



**Figure 2**  
A view, down the *b* axis, of the packing. Hydrogen bonds are indicated by dashed lines.

layers by intermolecular C9—H9 $\cdots$ O2<sup>i</sup> and C17—H17B $\cdots$ F<sup>ii</sup> interactions [symmetry codes: (i)  $2 - x, 1 - y, 1 - z$ ; (ii)  $x - 1, y, 1 + z$ ] (Fig. 2 and Table 2). The packing is further stabilized by  $\pi$ - $\pi$  interactions between the benzene (C2—C7) rings, the distance between the centroids, Cg $\cdots$ Cg<sup>iii</sup> [symmetry code: (iii)  $2 - x, -1 - y, -z$ ], being 3.713 Å.

## Experimental

To a solution of 3-(4-hydroxy-3-methoxyphenyl)acrylic acid (1.94 g, 0.01 mol) in 17.0% KOH solution (10 ml) was added dropwise 1-bromoheptane (0.54 g, 0.03 mol) in ethanol (30 ml). The mixture was heated under reflux for 24 h and extra KOH solution was added to remove the by-products. The mixture was then acidified to give a white precipitate, which was filtered and recrystallized from ethanol, giving a white precipitate, identified as 4-hydroxy-3-methoxyphenylacrylic acid. This compound (1.46 g) and DCC (1,3-dicyclohexylcarbodiimide, 0.6 g) were dissolved in THF (20 ml), and a solution of 2-fluoro-4-hydroxybenzotrile (0.68 g) and DMAP (4-dimethylaminopyridine, 0.01 g) in THF (20 ml) was added. The mixture was stirred at room temperature for 24 h and then filtered. Colorless single crystals of (I) suitable for X-ray diffraction study were obtained by slow evaporation of an ethyl acetate/petroleum ether (1:4 v/v) solution over a period of 2 d.

### Crystal data

C<sub>24</sub>H<sub>26</sub>FNO<sub>4</sub>  
M<sub>r</sub> = 411.46  
Triclinic, P1  
*a* = 7.763 (4) Å  
*b* = 11.207 (5) Å  
*c* = 13.631 (7) Å  
 $\alpha$  = 82.499 (8)°  
 $\beta$  = 82.269 (8)°  
 $\gamma$  = 75.662 (8)°  
*V* = 1132.6 (10) Å<sup>3</sup>

*Z* = 2  
*D<sub>x</sub>* = 1.207 Mg m<sup>-3</sup>  
Mo K $\alpha$  radiation  
Cell parameters from 2069 reflections  
 $\theta$  = 2.5–25.9°  
 $\mu$  = 0.09 mm<sup>-1</sup>  
*T* = 293 (2) K  
Column, colorless  
0.31 × 0.30 × 0.14 mm

### Data collection

Siemens SMART 1000 CCD area-detector diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T*<sub>min</sub> = 0.973, *T*<sub>max</sub> = 0.988  
5944 measured reflections

4124 independent reflections  
3035 reflections with *I* > 2 $\sigma$ (*I*)  
*R*<sub>int</sub> = 0.014  
 $\theta$ <sub>max</sub> = 25.5°  
*h* = -9 → 8  
*k* = -13 → 13  
*l* = -14 → 16

### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.057  
*wR*(*F*<sup>2</sup>) = 0.160  
*S* = 1.06  
4124 reflections  
283 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0764P)^2 + 0.2038P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
( $\Delta/\sigma$ )<sub>max</sub> < 0.001  
 $\Delta\rho$ <sub>max</sub> = 0.23 e Å<sup>-3</sup>  
 $\Delta\rho$ <sub>min</sub> = -0.21 e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

F—C7	1.329 (3)	O3—C17	1.423 (2)
F'—C3	1.291 (5)	O4—C14	1.366 (2)
O1—C8	1.369 (2)	O4—C18	1.439 (2)
O1—C5	1.393 (2)	N—C1	1.144 (3)
O2—C8	1.193 (2)	C8—C9	1.457 (3)
O3—C13	1.365 (2)	C9—C10	1.332 (3)

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C9—H9 $\cdots$ O2 <sup>i</sup>	0.93	2.58	3.509 (3)	177
C10—H10 $\cdots$ O1	0.93	2.35	2.730 (3)	104
C17—H17B $\cdots$ F <sup>ii</sup>	0.96	2.51	3.211 (4)	130

Symmetry codes: (i)  $-x + 2, -y + 1, -z + 1$ ; (ii)  $x - 1, y, z + 1$ .

All H atoms except H3 and H7 were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C) or *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(methyl C).

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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