The title compound (Fig. 1, DU-6859) is a new fluoroquinolone under development for use as an antimicrobial drug. Its antibacterial activity is significantly better than those of other quinolones. Those quinolone compounds have asymmetric carbons which play an important role in exhibiting the activity. DU-6859 has three asymmetric carbons; their configurations were estimated using chemical synthetic root based on the configuration of intermediates. However, there was no direct proof. In order to confirm the configuration, an X-ray analysis of the compound was undertaken.

A crystal used for X-ray analysis was recrystallized from acetonitrile. The crystal used for measurements was yellowish prismatic, and its size was approximately 0.4×0.25×0.25 mm³.

The intensity data (2θ<120°) were collected in the ω-2θ scan mode using graphite-monochromated Cu Kα radiation (λ=1.54178 Å). The data were corrected for Lorentz, polarization and absorption effects; 1388 unique reflections were used for the calculation. Bijvoet reflections were also measured. The crystal and experimental details are listed in Table 1.

The structure was solved by a direct method using the program SIR88. A full-matrix least-squares method was applied to the refinement. All non-hydrogen atoms were refined anisotropically. The highest peak in the final D-Fourier map was 0.15 eÅ⁻³. The final positional parameters are listed in Table 2, and the bond distances and angles are summarized in Tables 3 and 4.
An ORTEP drawing is shown in Fig. 2, and the molecular packing is shown in Fig. 3.

The absolute configuration was judged by comparing the differences of 132 Bijvoet pairs with a large difference. The number of Bijvoet pairs with the same signs of $|F_c(+) - F_c(-)|$ and $|F_o(+) - F_o(-)|$ was 129, which indicated the validity of the determined configuration. Consequently, the absolute configuration of the asymmetric carbons (C10, C11 and C16) proved to be $R$, $S$, and $S$, respectively. The molecule exists as a neutral form, though a zwitterionic form is probable because of the coexistence of acidic and basic groups. This is due to the presence of an intramolecular hydrogen bond between the carboxyl group and the carbonyl group in the quinoline ring [O1–O2: 2.53 Å, O1–H: 1.55 Å, H–O2: 1.03 Å, ∠O1–H–O2: 156˚].

### References


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