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Structure of (+)-Epigriseofulvin*

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In connection with our studies on both the microbial transformation of dehydrogriseofulvin analogs and the structure-activity relation of griseofulvin derivatives in their action on microtubules, it was necessary to determine the crystal structure of (+)-epigriseofulvin (1), since the structures of the C rings of 1 and (+)-griseofulvin (2) were used as the standard conformations in the elucidation of the structures of many related derivatives.

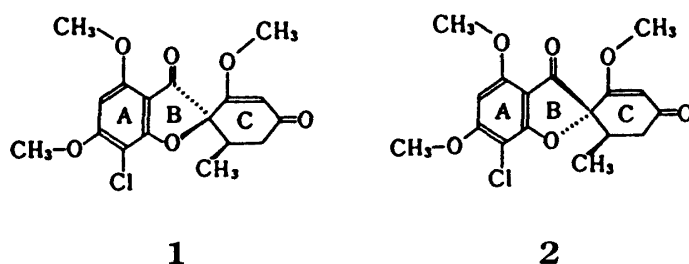


Chart 1.

The crystal and molecular structure of 1 were elucidated by X-ray structure analysis. The crystal belongs to a triclinic space group P1, with the unit cell parameters of $a=11.718$ (4), $b=9.800$ (3), $c=9.870$ (3) Å, $\alpha=103.49$ (3), $\beta=102.38$ (3), $\gamma=96.26$ (3)°, $v=1061$ (1) Å³. The unit cell contains two crystallographically independent 1 molecules and two chloroform molecules. The structure was solved by the direct method and refined to an R-value of 0.093 for 3971 non-zero reflections. No significant conformational differences between the two molecules were observed. The cyclohexenone rings take half-chair conformations with planar conjugated enone systems.

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