慶應義塾大学学術情報リポジトリ
Keio Associated Repository of Academic resouces

Title	Structure of (+)-epigriseofulvin
Sub Title	
Author	板井, 昭子(Itai, Akiko) 飯高, 洋一(Iitaka, Yoichi) 中村, 涼美(Nakamura, Suzumi) 小田, 泰子(Oda, Taiko) 佐藤, 良博(Sato, Yoshihiro)
Publisher	共立薬科大学
Publication year	1985
Jtitle	共立薬科大学研究年報 (The annual report of the Kyoritsu College of Pharmacy). No.30 (1985.) ,p.104- 104
JaLC DOI	
Abstract	
Notes	抄録
Genre	Technical Report
URL	https://koara.lib.keio.ac.jp/xoonips/modules/xoonips/detail.php?koara_id=AN00062898-00000030-0104

慶應義塾大学学術情報リポジトリ(KOARA)に掲載されているコンテンツの著作権は、それぞれの著作者、学会または出版社/発行者に帰属し、その権利は著作権法によって保護されています。引用にあたっては、著作権法を遵守してご利用ください。

The copyrights of content available on the KeiO Associated Repository of Academic resources (KOARA) belong to the respective authors, academic societies, or publishers/issuers, and these rights are protected by the Japanese Copyright Act. When quoting the content, please follow the Japanese copyright act.

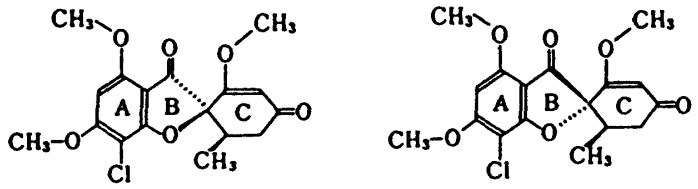
No. 30 (1985)

Structure of (+)-Epigriseofulvin*

Akiko ITAI**, Yoichi IITAKA**, Suzumi NAKAMURA, Taiko ODA and Yoshihiro SATO

板井昭子**, 飯高洋一**, 中村涼美, 小田泰子, 佐藤良博

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 microtublues, 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.



1 **2**

Chart 1.

The crystal and molecular structure of **1** were elucidated by X-ray structure analysis. The crystal belongs to a triclinic space group Pl, with the unit cell parameters of a=11.718 (4), b=9.800 (3), c=9.870 (3)Å, α=103.49 (3), β=102.38 (3), γ=96.26 (3)°, v=1061 (1)A^3. 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.

* 本報告は *Chem. Pharm. Bull.*, 33 (1), 158—164 (1985) に発表

** 東京大学薬学部