that available through the CIS, and the input is nearly identical. To illustrate the use and structure of the files, we give two examples of the input and results obtained.

The bibliographic file consists of all pertinent bibliographic information for each of the compounds contained in the file. It is thus possible to search for compound names, authors, and elemental composition as well as certain classes of compounds. A typical query might be phrased as follows: Q *AUTHOR "HUFFMAN" OR "WILSON" AND *FORMUL "C20-22" AND "O2-4" The above question would list the "REFCODES" for all compounds in the CCDF which contained between 20 and 22 carbons and two to four oxygens and which were authored by either Huffman or Wilson.

The connectivity file use is illustrated by the formulation of the search question for substructure **27** shown below:

```
Q CONNECTIVITY SEARCH FOR C8N RING

    ALLBOND C
    NOLN
    AT1 N 2
    AT2 C 2
    AT3 C 2
    AT4 C 2
    AT5 C 2
    AT6 C 2
    AT7 C 2
    AT8 C 2
    AT9 C 2
    BO 1 2 1
    BO 2 3 1
    BO 3 4 1
    BO 4 5 1
    BO 5 6 2
    BO 6 7 1
    BO 7 8 1
    BO 8 9 1
    BO 1 9 1
    END
```

The input consists of the question identifier (Q CONNECTIVITY), followed by the keywords "ALLBOND C" and "NOLN". The first indicates that all bonds identified by the bonding cards (BO n_1 n_2 ...) are cyclic in nature. This information could have been entered on the individual bonding cards if in fact some of the bond types were to be acyclic. The "NOLN" card indicates that for the fragment requested, no bonds are allowed between any of the designated atoms other than those specified.

Following these cards, the individual atoms are identified by using the atom cards. The general form of the atom card is ATn_1 n_2 n_3 n_4 n_5, where n_1 is the sequence number as referenced by the bonding cards, n_2 identifies the element (carbon or nitrogen in our example), n_3 is the number of connectives which will be given in the bonding table, and n_4 and n_5, when present, indicate the number of hydrogens present and the number of functional groups allowed. In the coding for **27** all atoms are specified only as being connected to two other atoms, and n_4 and n_5 are omitted. This will allow any type of functional group to be present on the atoms (i.e., H or R).

Once the atoms are specified, the bonding pattern is given. The bonding card format is BO n_1 n_2 n_3 n_4, where n_1 and n_2 indicate which atoms are to be connected, n_3 indicates the type of bond (1 = single bond, 2 = double bond, etc.), and n_4 indicates whether the bond is cyclic or acyclic. In the example given all bonds are single with the exception of the C5–C6 bond which is required to be double.

Once the connectivity search is run, a list of "REFCODES" is again generated. At this stage one can do one of three things with the REFCODE file. Complete bibliographic data can be obtained, plots of the molecule can be generated off-line (see Figure 2a), or the crystallographic data for the compounds can be extracted and data tapes created for later use. We point out here that the CCDF which is available through the NIH-EPA CIS system will perform most of the functions thus far discussed, although a terminal capable of recording data would be necessary in order to retrieve the crystallographic data for later use.

The system in use at the IUMSC creates a local "standard data tape" (SDT) which is identical in format with those used as input to all crystallographic programs in our library. Thus it is possible to search the CCDF for molecules of interest and then manipulate, plot, or examine them by using the crystallography programs.

The BMFIT program which generated Figure 3D is a local version of Nyburg's[28] BMFIT and differs only in that the "thermal" parameter usually drawn in crystallography programs is scaled so that the size of the "atom" is proportional to the deviation from one atom to the corresponding atom in the other molecule. The program itself transforms the crystallographic coordinates of one molecule to the unit cell of the other and then translates and rotates the first molecule so that the square of the distances between corresponding atoms is minimized.

Problems can occur when molecules contain "flexible" groups such as the furan in Figure 3A,B. In order to overcome the gross errors which would occur in such cases, two local programs, GENCART and CART21, were written to allow manipulation of the crystallographic parameters. GENCART transforms the crystallographic data to a set of molecular parameters so that the atoms are described as a series of distances, angles, and torsion angles. CART21 will then allow manipulation of any of these parameters and will generate a new data tape with the "adjusted" molecule transformed back to crystallographic coordinates (Figure 3C). CART21 can also be used to generate and add molecular fragments to existing molecules or to generate hypothetical molecules.

Acknowledgment. We wish to thank the National Institutes of Health (Grant No. GM-24438) for partial support of this work and the Marshal H. Wrubel Computer Center for computing time.

Synthesis of (24*R*,28*R*)- and (24*S*,28*S*)-Fucosterol Epoxides. Revision of C-24,28 Configurations[1]

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Received November 15, 1978

A facile synthesis of (24*R*,28*R*)- and (24*S*,28*S*)-24,28-epoxyfucosterol from fucosterol via the 24,28-glycols is described. The C-24,28 configurations were established by chemical correlation with sitosterol and clionasterol and show that previous assignments should be corrected.

Fucosterol epoxide (**1**) is a key intermediate in the dealkylation of sitosterol to cholesterol in insects.[2] For the detailed investigation of the mechanism of this dealkylation, it became necessary to develop a large-scale synthetic

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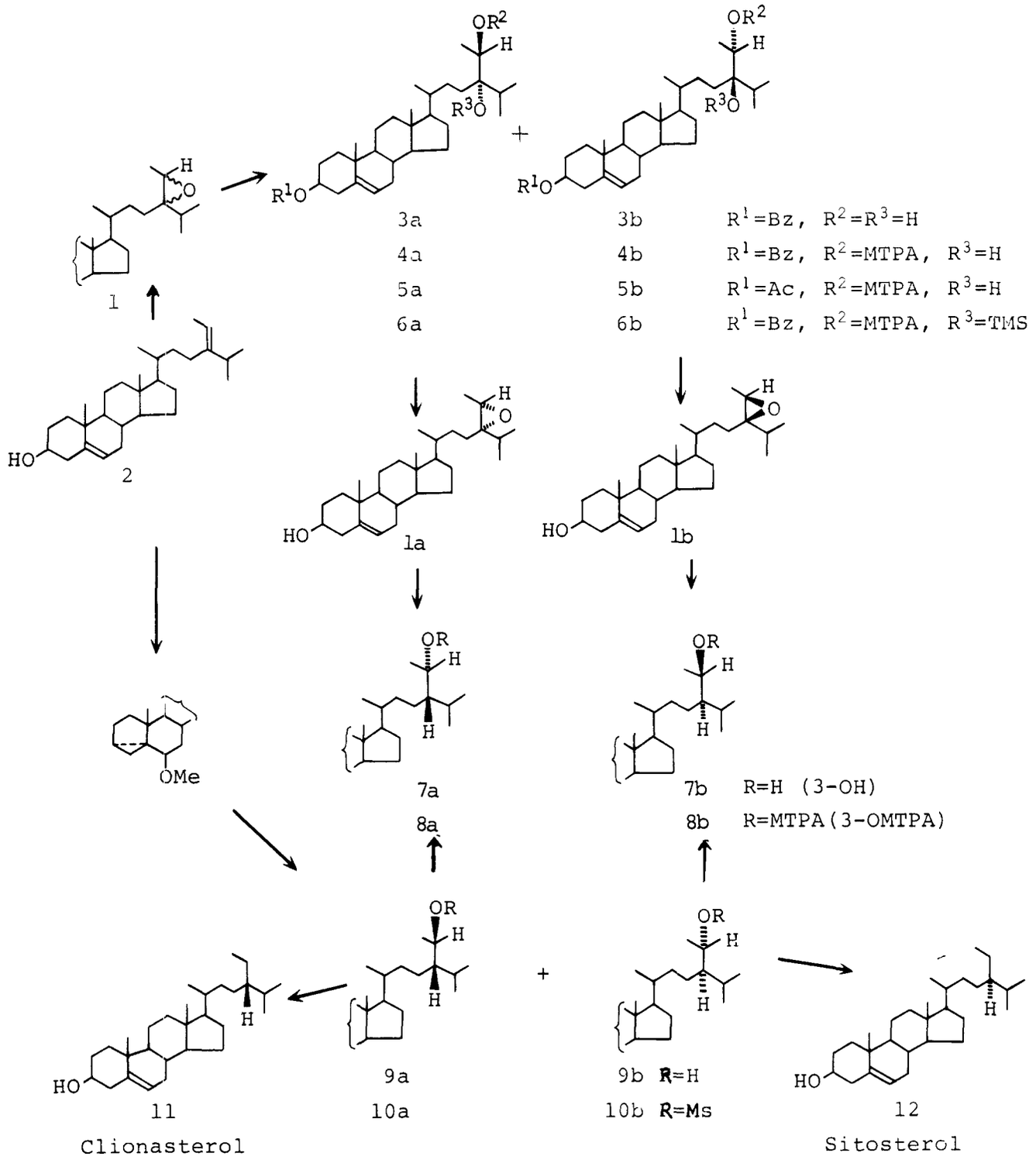

procedure with a defined stereochemical course. In a previous paper,[3] we have described the synthesis of both the (24S,28S)-**1a** and (24R,28R)-**1b** epoxides and demonstrated that only the former was converted to desmosterol in significant yield upon incubation with a cell-free system prepared from the midguts of the silkworm *Bombyx mori*.[4]

It was concluded that the (24S,28S)-epoxide is the actual intermediate of sitosterol dealkylation. However, subsequent studies indicated that the stereochemical assignment made in that work[3] needs revision. In this paper, we describe an improved synthesis of **1a** and **1b** and an unequivocal determination of their configurations.

Fucosterol (**2**) benzoate was treated with *m*-chloroperbenzoic acid (1.2 equiv) to give a 1:1 diastereomeric mixture (Figure 1) of the 24,28-epoxides in 72% yield. Acid-catalyzed ring opening of the epoxide gave the 24,28-glycol **3** in 70% yield. Neither the epoxide nor the 24,28-diol

(1) Studies on Steroids. 58. Part 57: M. Ishiguro, A. Akaiwa, Y. Fujimoto, S. Sato, and N. Ikekawa, *Tetrahedron Lett.*, 763 (1979).

(2) M. Morisaki, H. Ohotaka, M. Okubayashi, N. Ikekawa, Y. Horie, and S. Nakasone, *J. Chem. Soc., Chem. Commun.*, 1275 (1972).

(3) S.-M. L. Chen, K. Nakanishi, N. Awata, M. Morisaki, N. Ikekawa, and Y. Shimizu, *J. Am. Chem. Soc.*, **97**, 5297 (1975); S.-M. L. Chen, Ph.D. Thesis, Columbia University, 1975.

(4) N. Awata, M. Morisaki, and N. Ikekawa, *Biochem. Biophys. Res. Commun.*, **64**, 157 (1975).

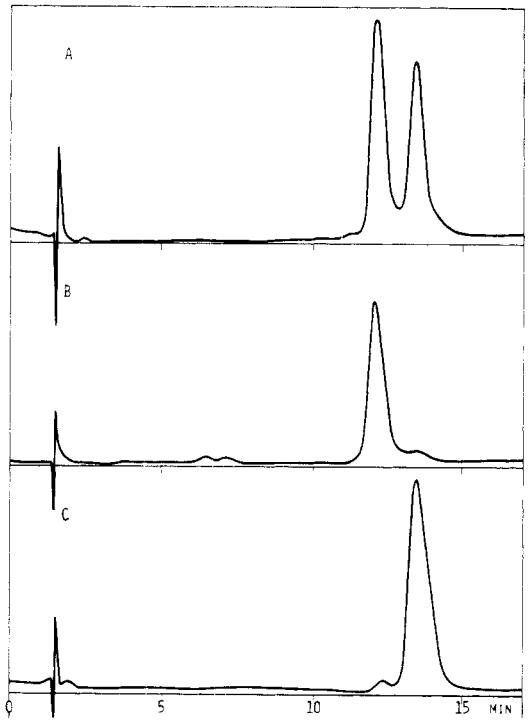

Figure 1. High-pressure LC of fucosterol epoxide benzoates: A, epoxide 1 obtained by epoxidation of fucosterol benzoate; B, epoxide **1b** derived from the more polar MTPA ester **4b**; C, epoxide **1a** derived from the less polar MTPA ester **4a**. Column, Zorbax SIL (25 cm × 2.1 mm i.d.); pressure, 90 kg/cm^2; solvent, hexane–CH_2Cl_2 (6:1).

mixtures could be resolved completely by thin-layer chromatography (TLC). Among several derivatives studied the 28-[(+)-α-methoxy-α-(trifluoromethyl)phenylacetyl] (MTPA) 3-benzoate **4** was found to be suitable for the resolution of the 24,28-diols. The corresponding 3-acetate **5** was previously[3] resolved by high-pressure liquid chromatography (LC) using Corasil II after being recycled five times.[5] Recrystallization of the MTPA benzoates **4** from ether gave the crystalline, less polar compound **4a**,[6] mp 89–90 °C, while the mother liquor contained mainly the more polar isomer **4b**. Treatment of the mother liquor with (trimethylsilyl)imidazole–trimethylchlorosilane gave the 24-(Me_3Si) ether **6**, and this derivative could be effectively resolved on TLC to afford pure **6b**, which on acid treatment regenerated **4b**. Treatment of pure **4a** and **4b** with 5% methanolic KOH gave the epoxides **1a** and **1b**, respectively, in 90% yields. The purity (>97% for each isomer) of **1a** and **1b** was ascertained by high-pressure LC analysis of the corresponding benzoates as shown in Figure 1.

The configurations of **1a** and **1b** were previously determined from the CD spectra of the Pr(dpm)$_3$ complexes[7] of the diols **3a** and **3b** (3-OH). To check the conclusions arrived at in that work,[3] we have reexamined the stereochemistry of **1a** and **1b** by a different route. Reduction of epoxides **1a** and **1b** with $LiAlH_4$–$AlCl_3$ (1:3) gave the 28-hydroxy alcohols **7a** and **7b**, respectively, together with the 24-hydroxy alcohols. During this reaction which yielded **7**, the configuration at C-24 is expected to be inverted, with retention of the C-28 configuration.[8] The stereochemistry of the alcohol **7b** derived from the less polar epoxide **1b** was determined as its bis(MTPA) ester **8b** by comparison with an authentic sample prepared as follows. The configuration of **7a** derived from the more polar epoxide **1a** was also determined by the same method.

The diastereoisomeric pair of 28-hydroxy alcohols of established configurations, (24*S*,28*R*)-**9a** and (24*R*,28*S*)-**9b**, were prepared from the 6β-methoxy-3,5-cyclo derivative of fucosterol by hydroboration–oxidation.[9] Their configurations at C-28 were deduced by a modification of Horeau's method and were determined by conversions of **9a** and **9b** to clionasterol (**11**) and sitosterol (**12**), respectively, as reported in our previous paper.[9] The configuration at C-28 in **9b** was inverted by treatment of the corresponding mesylates **10** with potassium superoxide.[10] Subsequent MTPA esterification of the C-28 hydroxyl group, acid treatment, and further MTPA esterification of the C-3 hydroxyl group afforded the 24*R*,28*R* bis(MTPA) ester **8b** in 40% yield from **9b**. The C-28 methyl signal of **8b** appeared at the same position, 1.26 ppm, as that of the sample derived from the less polar epoxide **1b**. By the same procedure, **9a** could be converted to **8a** which showed the C-28 methyl signal at 1.36 ppm. Further evidence for identification of **8a** and **8b** was obtained from high-pressure LC analysis, which showed identical mobilities for the compounds derived from **1a** and **9a** and **1b** and **9b**, respectively, as shown in Figure 2.[11]

Thus the stereochemistries of the bis(MTPA) esters **8a** and **8b** were established as 24*S*,28*S* and 24*R*,28*R*, respectively; this leads to a 24*S*,28*S* configuration for the more polar epoxide **1a** and a 24*R*,28*R* configuration for the less polar epoxide **1b**. These assignments are opposite the previous conclusions.[3]

In the previous paper,[3] the absolute configurations of the 24,28-glycols **3a** and **3b** (3-OH) were assigned on the basis of the CD spectra of their Pr(dpm)$_3$ complexes. However, from the evidence presented above, it can be concluded that there was an error in the assignment of the most stable conformation of the complex formed between Pr(dpm)$_3$ and the acyclic *sec*-/*tert*-glycol system.

We have since found that the two epoxides **1a** and **1b** (3-OH) are both formed in vitro (silkworm gut) and in vivo (fifth instar of silkworm larvae) in approximately the same yield. Details of this aspect and the conversion of both epoxides to desmosterol in insects will be published elsewhere.[12]

Experimental Section

^{1}H NMR spectra (60 MHz) were recorded on a Hitachi R-24A spectrometer in deuteriochloroform solution with tetramethylsilane as internal standard. A Shimadzu Du Pont Model 830 liquid chromatograph equipped with a UV detector (254 nm) was used with a Zorbax SIL column, 25 cm × 2.1 mm i.d. Column chromatography was normally effected with Wako silica gel C-200. "The usual workup" refers to dilution with water, extraction with

(5) Stereochemical interrelationships of the previously[3] prepared acetates **5a** and **5b** to the presently synthesized benzoates **4a** and **4b** rest on (i) the relative mobility on TLC and high-pressure LC (**4a** and **5a** are less polar than **4b** and **5b**, respectively), (ii) the coincidence of the C-29 methyl ^{1}H NMR signal (**4a** and **5a**, 1.26 ppm; **4b** and **5b**, 1.36 ppm), and (iii) the identical melting points of the triols derived from **4a** and **5a**, 168–170 °C, and those of the diastereoisomeric triols derived from **4b** and **5b**, 174–176 °C.

(6) In this paper, "a" refers to a series of compounds which can be connected to the more polar epoxide benzoate (**1a** benzoate) and "b" to the less polar one (**1b** benzoate).

(7) K. Nakanishi, D. A. Schooley, M. Koreeda, and J. Dillon, *Chem. Commun.*, 1235 (1971); J. Dillon and K. Nakanishi, *J. Am. Chem. Soc.*, **96**, 4057, 4059 (1974).

(8) H. O. House, "Modern Synthetic Reactions", 2nd ed., W. A. Benjamin, Menlo Park, CA, 1972, p 103.

(9) Y. Fujimoto and N. Ikekawa, *J. Org. Chem.*, **44**, 1011 (1979).

(10) E. J. Corey, K. C. Nicolaou, M. Shibasaki, Y. Machida, and C. S. Shiner, *Tetrahedron Lett.*, 3183 (1975).

(11) It was also found that **8a** was clearly distinguished from the 24*R*,28*S* bis(MPTA) ester derived from **9b** by high-pressure LC. This fact confirmed the above-mentioned stereochemical course, yielding **7a** from **1a**.

(12) Y. Fujimoto, M. Morisaki, and N. Ikekawa, submitted for publication in *Biochemistry*.

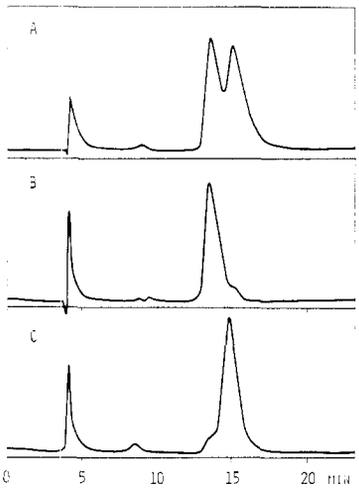

Figure 2. High-pressure LC of the bis(MTPA) esters of stigmast-5-ene-3β,28-diol (**8a** and **8b**): A, a mixture of bis(MTPA) esters **8a** and **8b** obtained from **9a** and **9b**, respectively (retention time: **8a**, 13.4 min; **8b**, 15.1 min); B, bis(MTPA) ester from the epoxide **1b**; C, bis(MTPA) ester from the epoxide **1a**. Column, Zorbax SIL (25 cm × 2.1 mm i.d.); pressure, 80 kg/cm^2; solvent, hexane–CH_2Cl_2 (10:1).

an organic solvent, washing to neutrality, drying over $MgSO_4$, filtration, and evaporation of solvent under vacuum.

24,28-Epoxystigmast-5-en-3β-ol 3-Benzoate (1) (Isomeric Mixture). To a solution of 4.3 g of fucosterol benzoate (**2**-BzO) in 100 mL of chloroform was added 1.72 g of *m*-chloroperbenzoic acid at −20 °C, and the mixture was stirred for 20 min. After addition of dilute NaOH to make the mixture alkaline, the mixture was extracted with $CHCl_3$. After the usual workup, the crude product was chromatographed on silica gel. From the fraction eluted with hexane–benzene (2:1), the starting **2**-BzO (1.0 g) was recovered, and the fraction eluted with benzene afforded 3.2 g of the epoxide **1**: mp 134–142 °C (from methanol); NMR δ 0.7 (3 H, s, 18-Me), 1.25 (3 H, d, J = 6 Hz, 29-Me), 2.9 (1 H, q, J = 6 Hz, 28-H), 4.9 (1 H, m, 3-H), 5.4 (1 H, m, 6-H), 7.3–8.2 (5 H, m, aromatic).

Stigmast-5-ene-3β,24,28-triol 3-Benzoate (3) (Isomeric Mixture). A mixture of 3.1 g of the epoxide **1**, 65 mL of tetrahydrofuran (THF), 1 mL of H_2O, and 0.2 mL of concentrated H_2SO_4 was stirred overnight at room temperature. The product was chromatographed on silica gel. Elution with benzene–ethyl acetate (20:1) afforded 2.3 g of the glycol **3**: mp 170–172 °C (from methanol); NMR δ 0.7 (3 H, s, 18-Me), 1.20 (3 H, d, J = 6 Hz, 29-Me), 3.8 (1 H, m, 28-H), 4.9 (1 H, m, 3-H), 5.4 (1 H, m, 6-H), 7.3–8.2 (5 H, m, aromatic).

28-MTPA Ester of (24S,28R)-3β-Benzoylstigmast-5-ene-24,28-diol (4a). A mixture of 1.8 g of the glycol **3**, 12 mL of pyridine, and 1.5 mL of (+)-α-methoxy-α-(trifluoromethyl)-phenylacetyl chloride (MTPAC) was stirred at room temperature overnight. The usual workup gave 2.4 g of the crude MTPA ester **4**, which was crystallized from ether to give 1.1 g of **4a**: mp 88–91 °C; NMR δ 0.66 (3 H, s, 18-Me), 1.27 (3 H, d, J = 6 Hz, 28-Me), 3.5 (3 H, s, MeO), 4.9 (1 H, m, 3-H), 5.15 (1 H, q, J = 6 Hz, 28-H), 5.45 (1 H, m, 6-H), 7.3–8.2 (10 H, m, aromatic).

28-MTPA Ester of (24R,28S)-3β-Benzoylstigmast-5-ene-24,28-diol (4b). A mixture of the mother liquor of the above crystallization, 0.8 mL of (trimethylsilyl)imidazole, and 200 μL of trimethylchlorosilane was heated at 110 °C for 2 h under argon, cooled, and diluted with ether. The usual workup gave the crude Me_3Si ether, which was developed by TLC two times with hexane–benzene (3:2). Elution of the band with R_f 0.6 with ethyl acetate gave 180 mg of **6b**: NMR δ 0.16 (9 H, s, Me_3Si), 0.66 (3 H, s, 18-Me), 1.34 (3 H, d, J = 6 Hz, 29-Me), 3.60 (3 H, s, MeO), 4.9 (1 H, m, 3-H), 5.1 (1 H, m, 28-H), 5.4 (1 H, m, 6-H), 7.3–8.2 (10 H, m, aromatic). A mixture of 120 mg of **6b**, 20 mL of THF, and 5 drops of 1 N HCl was stirred at room temperature overnight. The usual workup gave 100 mg of **4b** as an oil: NMR δ 0.66 (3 H, s, 18-Me), 1.36 (3 H, d, J = 6 Hz, 29-Me), 3.5 (3 H, s, MeO), 4.9 (1 H, m, 3-H), 5.15 (1 H, q, J = 6 Hz, 28-H), 5.45 (1 H, m, 6-H), 7.3–8.2 (10 H, m, aromatic).

(24S,28S)- and (24R,28R)-24,28-Epoxystigmast-5-en-3β-ol (1a and 1b). A mixture of 500 mg of **4a**, 5% methanolic KOH (20 mL), and THF (15 mL) was stirred at room temperature for 12 h, and the usual workup followed by crystallization from methanol gave 250 mg of **1a**: mp 143–145 °C; NMR δ 0.7 (3 H, s, 18-Me), 1.22 (3 H, d, J = 6 Hz, 29-Me), 2.8 (1 H, q, J = 6 Hz, 28-H), 3.5 (1 H, m, 3-H), 5.4 (1 H, m, 6-H). In the same manner, 120 mg of **1b** was obtained from 250 mg of **4b**; mp 121 °C (from methanol). The NMR of **1b** was identical with that of **1a**, and the two compounds could not be distinguished by their NMR spectra.

Bis(MTPA) Ester of (24R,28R)-Stigmast-5-ene-3β,28-diol (8b). (A) From the Epoxide 1b. To a suspension of 120 mg of $LiAlH_4$ and 400 mg of $AlCl_3$ in 3 mL of dry ether was added 100 mg of the epoxide **1b** in 12 mL of dry ether. The mixture was refluxed under argon for 2 h. After the mixture was cooled, excess reagent was destroyed by addition of wet ether. The usual workup gave a mixture of the 28- and 24-hydroxy compounds, which was directly treated with 1 mL of pyridine and 100 μL of MTPAC at room temperature for 2 h. The usual workup and chromatography of the crude product with benzene–ethyl acetate (50:1) gave 62 mg of the bis(MTPA) ester **8b**: NMR δ 0.7 (3 H, s, 18-Me), 1.26 (3 H, d, J = 6 Hz, 29-Me), 3.55 (6 H, s, 2 MeO), 4.9 (1 H, m, 3-H), 5.2 (1 H, m, 28-H), 5.4 (1 H, m, 6-H), 7.3–7.8 (10 H, m, aromatic). Further elution with benzene–ethyl acetate (40:1) afforded 55 mg of the 3-MTPA ester of stigmast-5-ene-3β,24-diol: NMR δ 0.7 (3 H, s, 18-Me), 3.57 (3 H, s, MeO), 4.9 (1 H, m, 3-H), 5.4 (1 H, m, 6-H), 7.3–7.7 (5 H, m, aromatic).

(B) From the 28-Hydroxy Compound 9b. A mixture of 45 mg of (24R,28S)-6β-methoxy-3,5-cyclostigmastan-28-ol (**9b**), 100 μL of methanesulfonyl chloride, and 1 mL of pyridine was stirred at room temperature for 3 h. The usual workup gave 55 mg of the crude mesylate: NMR δ 1.4 (3 H, d, J = 6 Hz, 29-Me), 2.75 (1 H, m, 6-H), 2.96 (3 H, s, MePh), 3.29 (3 H, s, MeO), 4.9 (1 H, m, 28-H). A mixture of the mesylate, 2.4 mL of dimethyl sulfoxide, 2.4 mL of dimethylformamide, 24 mg of KO_2, and 120 mg of dicyclohexyl-18-crown-6 was stirred at room temperature for 3 h. The crude product obtained by the usual workup was chromatographed to give 38 mg of the 6β-methoxy-3,5-cyclo derivative of the (24R,28R)-28-hydroxy compound: NMR δ 0.70 (3 H, s, 18-Me), 1.33 (3 H, d, J = 6 Hz, 29-Me), 2.75 (1 H, m, 6-H), 3.30 (3 H, s, MeO), 3.55 (1 H, q, J = 6 Hz, 28-H). A solution of the alcohol in dioxane (2 mL) and H_2O (0.75 mL) was refluxed for 2 h in the presence of a catalytic amount of *p*-toluenesulfonic acid. The usual workup gave the mono MTPA ester: NMR δ 1.26 (3 H, d, J = 6 Hz, 29-H), 3.55 (3 H, s, MeO), 3.5 (1 H, m, 3-H), 5.4 (2 H, m, 28-H and 6-H), 7.3–7.8 (5 H, m, aromatic). The ester was treated with 40 μL of MTPAC and 2 mL of pyridine to give 38 mg of the bis(MTPA) ester **8b**. The NMR spectrum and the high-pressure LC mobility were completely identical with those of the sample obtained by procedure A.

Bis(MTPA) Ester of (24S,28S)-Stigmast-5-ene-3β,28-diol (8a). (A) From the Epoxide 1a. When 75 mg of the epoxide **1a** was treated in the same manner as that described for **1b**, 45 mg of the bis(MTPA) ester was obtained as an oil: NMR δ 0.7 (3 H, s, 18-Me), 1.36 (3 H, d, J = 6 Hz, 29-Me), 3.6 (6 H, s, 2 MeO), 4.9 (1 H, m, 3-H), 5.3 (1 H, m, 28-H), 5.4 (1 H, m, 6-H), 7.3–7.8 (10 H, m, aromatic).

(B) From the 28-Hydroxy Compound 9a. When 40 mg of (24S,28R)-28-hydroxy compound **9a** was treated in the same manner as that described for **9b**, 30 mg of the bis(MTPA) ester **8a** was obtained. The NMR spectrum and the high-pressure LC mobility were completely identical with those of the sample obtained by method A.

Acknowledgment. We thank Professor Koji Nakanishi, Columbia University, for helpful discussions throughout this work.

Registry No. **1a**, 55870-01-4; **1a** benzoate, 72317-97-6; **1b**, 57173-68-9; **1b** benzoate, 72376-61-5; **2** benzoate, 72317-98-7; **3a**, 69476-97-7; **3b**, 69500-94-3; **4a**, 69476-98-8; **4b**, 69500-95-4; **6b**, 72317-99-8; **8a**, 69477-00-5; **8b**, 69500-99-8; **9a**, 68889-64-5; **9b**, 68844-32-6; **10b**, 68844-33-7; (24S)-stigmast-5-ene-3β,24-diol 3-MTPA ester, 72318-00-4; (24R, 28R)-6β-methoxy-3,5-cyclostigmatan-28-ol, 71242-46-1; (24R, 28R)-6β-methoxy-3,5-cyclostigmastan-28-ol mono MTPA ester, 72330-99-5.