C17	−0.2739 (8)	−0.5323 (3)	−0.8207 (9)	0.064 (2)
C18	−0.1394 (5)	−0.4467 (2)	−0.3371 (7)	0.045 (2)
C19	0.1564 (5)	−0.4735 (2)	−0.2518 (7)	0.043 (2)
C20	0.2370 (6)	−0.5143 (3)	−0.356 (1)	0.063 (2)
C21	0.2767 (5)	−0.4234 (2)	−0.1542 (6)	0.044 (1)
C22	0.3278 (6)	−0.3189 (2)	−0.1425 (7)	0.048 (2)
C23	0.2979 (8)	−0.2780 (3)	−0.3174 (9)	0.063 (2)
C24	0.2996 (7)	−0.2925 (3)	0.0367 (8)	0.054 (2)
C25	0.333 (2)	−0.2081 (4)	0.231 (1)	0.110 (5)
O*W*	−0.9285 (6)	−0.4204 (3)	−0.7617 (6)	0.088 (2)

Table 2. *Geometric parameters* (Å, °)

O1—C7	1.478 (10)	N3—C21	1.332 (7)
O1—C8	1.329 (9)	N3—C22	1.466 (7)
O2—C8	1.210 (7)	C6—C7	1.492 (14)
O3—C18	1.234 (6)	C9—C10	1.518 (9)
O4—C21	1.224 (6)	C9—C11	1.571 (7)
O5—C24	1.187 (10)	C9—C18	1.538 (6)
O6—C24	1.304 (8)	C11—C12	1.506 (8)
O6—C25	1.435 (12)	C19—C20	1.512 (9)
N1—C8	1.359 (8)	C19—C21	1.534 (7)
N1—C9	1.452 (7)	C22—C23	1.508 (8)
N2—C18	1.332 (7)	C22—C24	1.510 (9)
N2—C19	1.454 (6)		
C7—O1—C8	111.2 (7)	N2—C18—C9	118.8 (5)
C24—O6—C25	118.1 (7)	O3—C18—C9	119.0 (7)
C8—N1—C9	120.4 (5)	O3—C18—N2	122.0 (6)
C18—N2—C19	122.7 (5)	N2—C19—C21	112.7 (5)
C21—N3—C22	122.5 (6)	N2—C19—C20	110.5 (5)
O1—C7—C6	107.4 (7)	C20—C19—C21	110.3 (6)
O2—C8—N1	125.3 (6)	N3—C21—C19	117.2 (5)
O1—C8—N1	112.3 (6)	O4—C21—C19	119.4 (5)
O1—C8—O2	122.4 (6)	O4—C21—N3	123.4 (6)
N1—C9—C10	110.9 (5)	N3—C22—C24	110.2 (6)
N1—C9—C11	108.4 (5)	N3—C22—C23	109.3 (5)
N1—C9—C18	111.8 (6)	C23—C22—C24	114.3 (5)
C11—C9—C18	106.2 (5)	O6—C24—C22	111.5 (6)
C10—C9—C18	111.1 (5)	O5—C24—C22	126.0 (6)
C10—C9—C11	108.4 (6)	O5—C24—O6	122.5 (7)
C9—C11—C12	116.3 (6)		

Program used to solve structure: *SHELXS*86 (Sheldrick, 1985). Structure refined by blocked full-matrix least squares with anisotropic thermal parameters for all non-H atoms. H atoms located on a ΔF map, but not refined. Program used to refine structure: *SHELX*76 (Sheldrick, 1976).

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55601 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CD1012]

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Tricyclo[9.3.0.0^{3,7}]tetradec-3-ene-5,10-dione (I), Tetracyclo[9.3.0.0^{1,5}.0^{5,9}]tetradecane-2,7-dione (II) and *cis-cisoid-cis*-2,9-Epoxy-9-methyltricyclo[9.3.0.0^{4,8}]tetradecan-2-ol (III)

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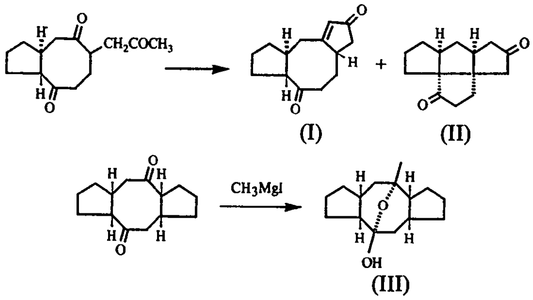
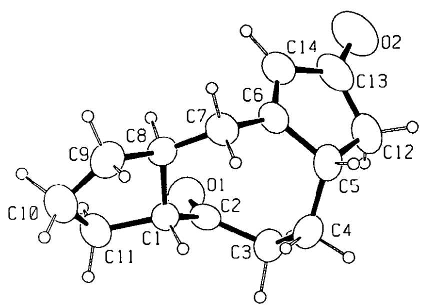
Abstract

The crystal structures of the three title compounds, which were obtained during studies of the preparation and reactions of 5–8–5 fused-ring compounds, have been determined by X-ray diffraction.

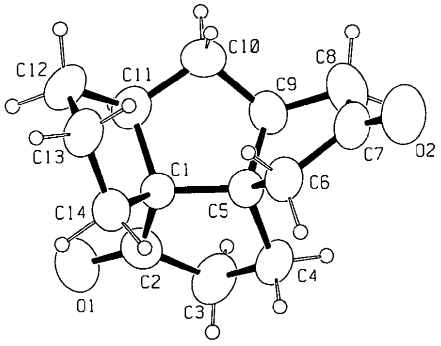
Comment

The syntheses of compounds (I)–(III) are reported separately (Umehara, Honnami, Hishida, Kawata, Ohba & Zen, 1992). The conformations of the cyclooctane rings in the related 5–8 or 5–8–5 fused-ring compounds have been investigated previously (Okumoto, Ohba, Saito, Ishii, Umehara & Hishida, 1987; Okumoto, Ohba, Saito, Umehara & Hishida, 1988; Umehara, Hishida, Okuda, Ohba, Ito, Saito & Zen, 1990). The eight-membered ring takes a boat–chair form in (I) and a boat–boat form in (III). There is an intermolecular hydrogen bond in (III), O(1)···O(2) $(1-x, -y, -z) = 2.838\ (2)$ Å.

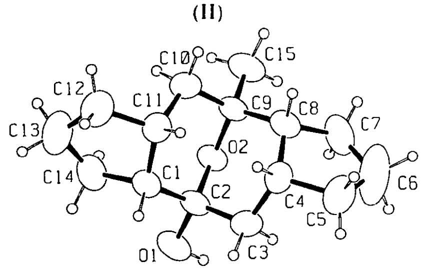




(I)



(II)



(III)

Fig. 1. *ORTEP* drawings (Johnson, 1965) of the molecules with 50% probability ellipsoids. H atoms are represented by circles of 0.08 Å radius.

Experimental

Compound (I)

Crystal data

$C_{14}H_{18}O_2$
$M_r = 218.3$
Triclinic
$P\overline{1}$
$a = 9.894$ (1) Å
$b = 10.971$ (2) Å
$c = 5.658$ (1) Å
$\alpha = 102.90$ (1)°
$\beta = 91.17$ (1)°
$\gamma = 81.14$ (1)°
$V = 591.5$ (1) Å^3
$Z = 2$

$D_x = 1.226$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 40 reflections
$\theta = 10$–15°
$\mu = 0.075$ mm^{-1}
$T = 298$ (2) K
Prism
0.50 × 0.30 × 0.10 mm
Colourless

Data collection

Rigaku AFC-5 four-circle diffractometer
θ–2θ scans
Absorption correction: by integration from crystal shape
$T_{\min} = 0.978$, $T_{\max} = 0.991$
2880 measured reflections
2720 independent reflections

1501 observed reflections [$|F_o| > 3\sigma|F_o|$]
$\theta_{\max} = 27.5°$
$h = -12 \rightarrow 0$
$k = -14 \rightarrow 14$
$l = -7 \rightarrow 7$
5 standard reflections monitored every 100 reflections intensity variation: 0.988–1.012

Refinement

Refinement on F
Final $R = 0.044$
$wR = 0.047$
$S = 1.79$
1501 reflections
218 parameters
All H-atom parameters refined

$w = [\sigma^2|F_o| + (0.015|F_o|)^2]^{-1}$
$(\Delta/\sigma)_{\max} = 0.109$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Compound (II)

Crystal data

$C_{14}H_{18}O_2$
$M_r = 218.3$
Monoclinic
$P2_1/a$
$a = 13.406$ (2) Å
$b = 13.346$ (2) Å
$c = 6.860$ (2) Å
$\beta = 104.61$ (2)°
$V = 1187.7$ (4) Å^3
$Z = 4$
$D_x = 1.221$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 24 reflections
$\theta = 10$–15°
$\mu = 0.075$ mm^{-1}
$T = 293$ (2) K
Prism
0.55 × 0.50 × 0.45 mm
Colourless

Data collection

Rigaku AFC-5 four-circle diffractometer
θ–2θ scans
Absorption correction: none
2948 measured reflections
2727 independent reflections
1128 observed reflections [$|F_o| > 3\sigma|F_o|$]

$\theta_{\max} = 27.5°$
$h = -17 \rightarrow 17$
$k = 0 \rightarrow 17$
$l = 0 \rightarrow 8$
5 standard reflections monitored every 100 reflections intensity variation: 0.976–1.050

Refinement

Refinement on F
Final $R = 0.050$
$wR = 0.046$
$S = 1.54$
1128 reflections
218 parameters
All H-atom parameters refined

$w = [\sigma^2|F_o| + (0.015|F_o|)^2]^{-1}$
$(\Delta/\sigma)_{\max} = 0.219$
$\Delta\rho_{\max} = 0.14$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Compound (III)

Crystal data

$C_{15}H_{24}O_2$
$M_r = 236.4$

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Monoclinic
$P2_1/n$
$a = 12.109$ (2) Å
$b = 10.649$ (2) Å
$c = 10.407$ (1) Å
$\beta = 98.30$ (1)°
$V = 1327.9$ (4) Å^3
$Z = 4$
$D_x = 1.182$ Mg m^{-3}

Cell parameters from 24 reflections
$\theta = 10$–15°
$\mu = 0.071$ mm^{-1}
$T = 298$ (2) K
Prism
0.40 × 0.40 × 0.30 mm
Colourless

Data collection

Rigaku AFC-5 four-circle diffractometer
θ–2θ scans
Absorption correction: by integration from crystal shape
$T_{\min} = 0.973$, $T_{\max} = 0.981$
3211 measured reflections
3138 independent reflections

1319 observed reflections $[|F_o|>3\sigma|F_o|]$
$\theta_{\max} = 27.5$°
$h = 0 \rightarrow 15$
$k = -13 \rightarrow 0$
$l = -13 \rightarrow 13$
5 standard reflections monitored every 100 reflections intensity variation: 0.990–1.006

Refinement

Refinement on F
Final $R = 0.048$
$wR = 0.050$
$S = 1.87$
1319 reflections
251 parameters
All H-atom parameters refined

$w = [\sigma^2|F_o|+(0.015|F_o|)^2]^{-1}$
$(\Delta/\sigma)_{\max} = 0.113$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.22$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$U_{\text{eq}} = \tfrac{1}{3}\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
(I)				
O1	0.6019 (2)	0.3516 (1)	1.0144 (2)	0.057
O2	1.0937 (2)	0.1619 (2)	1.0533 (3)	0.091
C1	0.5622 (2)	0.3064 (2)	0.5901 (3)	0.038
C2	0.6285 (2)	0.3702 (2)	0.8181 (3)	0.038
C3	0.7249 (2)	0.4614 (2)	0.8010 (4)	0.048
C4	0.8264 (2)	0.4252 (2)	0.5876 (4)	0.052
C5	0.9341 (2)	0.3085 (2)	0.5854 (4)	0.052
C6	0.8754 (2)	0.1880 (2)	0.5729 (3)	0.043
C7	0.7721 (2)	0.1464 (2)	0.3860 (3)	0.048
C8	0.6273 (2)	0.1671 (2)	0.4930 (3)	0.041
C9	0.5213 (3)	0.1182 (2)	0.3097 (4)	0.058
C10	0.3823 (3)	0.1880 (3)	0.4134 (5)	0.075
C11	0.4115 (2)	0.2945 (2)	0.6248 (4)	0.055
C12	1.0270 (2)	0.3157 (2)	0.8076 (5)	0.071
C13	1.0249 (2)	0.1946 (2)	0.8899 (4)	0.060
C14	0.9268 (2)	0.1259 (2)	0.7414 (4)	0.051
(II)				
O1	0.0305 (1)	0.2176 (2)	0.0474 (4)	0.082
O2	0.5661 (2)	0.1075 (2)	0.4541 (4)	0.104
C1	0.1894 (2)	0.1341 (2)	0.2125 (4)	0.039
C2	0.1232 (2)	0.2212 (2)	0.1100 (4)	0.055
C3	0.1880 (2)	0.3119 (2)	0.1005 (6)	0.073
C4	0.2969 (2)	0.2703 (2)	0.1314 (5)	0.056
C5	0.3006 (2)	0.1765 (2)	0.2650 (4)	0.042
C6	0.3898 (2)	0.1063 (2)	0.2528 (5)	0.054
C7	0.4777 (2)	0.1350 (2)	0.4315 (5)	0.069
C8	0.4389 (3)	0.2026 (3)	0.5726 (6)	0.088
C9	0.3227 (2)	0.2018 (2)	0.4930 (5)	0.057
C10	0.2669 (2)	0.1179 (2)	0.5734 (4)	0.063
C11	0.1640 (2)	0.1083 (2)	0.4175 (4)	0.049
C12	0.1177 (2)	0.0027 (2)	0.3909 (5)	0.062
C13	0.1669 (2)	−0.0466 (2)	0.2387 (5)	0.060
C14	0.1668 (2)	0.0365 (2)	0.0871 (4)	0.052
(III)				
O1	0.4471 (1)	0.1217 (2)	−0.1089 (2)	0.059
O2	0.6176 (1)	0.1128 (1)	0.0139 (2)	0.043
C1	0.5569 (2)	0.3026 (3)	−0.1053 (2)	0.045
C2	0.5232 (2)	0.1940 (2)	−0.0250 (2)	0.043
C3	0.4735 (2)	0.2286 (3)	0.0960 (3)	0.052
C4	0.5559 (2)	0.2901 (3)	0.2038 (3)	0.050
C5	0.5154 (3)	0.2818 (3)	0.3364 (3)	0.075
C6	0.5622 (4)	0.1648 (5)	0.3973 (4)	0.136
C7	0.6495 (3)	0.1151 (3)	0.3210 (3)	0.070
C8	0.6681 (2)	0.2189 (3)	0.2239 (3)	0.049
C9	0.7083 (2)	0.1752 (2)	0.0977 (2)	0.042
C10	0.7508 (2)	0.2830 (3)	0.0207 (3)	0.051
C11	0.6613 (2)	0.3752 (3)	−0.0415 (2)	0.049
C12	0.6994 (3)	0.4461 (3)	−0.1552 (3)	0.071
C13	0.6618 (3)	0.3679 (4)	−0.2759 (3)	0.094
C14	0.5882 (3)	0.2634 (3)	−0.2376 (3)	0.063
C15	0.7984 (2)	0.0755 (3)	0.1223 (3)	0.063

Table 2. *Geometric parameters* (Å, °)

(I)			
O1—C2	1.214 (2)	C5—C12	1.537 (3)
O2—C13	1.223 (3)	C6—C7	1.502 (3)
C1—C2	1.513 (2)	C6—C14	1.340 (3)
C1—C8	1.545 (2)	C7—C8	1.531 (3)
C1—C11	1.537 (3)	C8—C9	1.531 (3)
C2—C3	1.503 (3)	C9—C10	1.527 (3)
C3—C4	1.528 (3)	C10—C11	1.531 (3)
C4—C5	1.532 (3)	C12—C13	1.507 (4)
C5—C6	1.511 (3)	C13—C14	1.457 (3)
(II)			
O1—C2	1.209 (3)	C5—C9	1.554 (4)
O2—C7	1.212 (4)	C6—C7	1.520 (4)
C1—C2	1.523 (4)	C7—C8	1.508 (5)
C1—C5	1.549 (4)	C8—C9	1.516 (4)
C1—C11	1.567 (4)	C9—C10	1.525 (5)
C1—C14	1.547 (4)	C10—C11	1.523 (4)
C2—C3	1.501 (4)	C11—C12	1.533 (4)
C3—C4	1.526 (4)	C12—C13	1.518 (5)
C4—C5	1.545 (4)	C13—C14	1.521 (4)
C5—C6	1.538 (4)		
(III)			
O1—C2	1.404 (3)	C5—C6	1.474 (6)
O2—C2	1.443 (3)	C6—C7	1.506 (6)
O2—C9	1.460 (3)	C7—C8	1.536 (4)
C1—C2	1.516 (4)	C8—C9	1.538 (4)
C1—C11	1.548 (3)	C9—C10	1.531 (4)
C1—C14	1.539 (4)	C9—C15	1.517 (4)
C2—C3	1.517 (4)	C10—C11	1.534 (4)
C3—C4	1.536 (4)	C11—C12	1.530 (4)
C4—C5	1.532 (4)	C12—C13	1.521 (5)
C4—C8	1.544 (4)	C13—C14	1.514 (5)
(I)			
C2—C1—C8	113.3 (2)	C7—C6—C14	125.8 (2)
C2—C1—C11	114.0 (2)	C6—C7—C8	112.6 (1)
C8—C1—C11	102.1 (2)	C1—C8—C7	115.9 (2)
O1—C2—C1	121.0 (2)	C1—C8—C9	102.0 (2)
O1—C2—C3	119.8 (2)	C7—C8—C9	113.7 (2)
C1—C2—C3	119.2 (2)	C8—C9—C10	106.0 (2)
C2—C3—C4	117.5 (2)	C9—C10—C11	106.4 (2)
C3—C4—C5	115.6 (2)	C1—C11—C10	104.9 (2)
C4—C5—C6	114.2 (2)	C5—C12—C13	105.7 (2)
C4—C5—C12	115.9 (2)	O2—C13—C12	125.1 (2)
C6—C5—C12	103.3 (2)	O2—C13—C14	127.1 (2)
C5—C6—C7	121.6 (2)	C12—C13—C14	107.8 (2)
C5—C6—C14	112.6 (2)	C6—C14—C13	110.3 (2)

(II)

C2—C1—C5	104.1 (2)	C6—C5—C9	103.5 (2)
C2—C1—C11	110.4 (2)	C5—C6—C7	105.0 (2)
C2—C1—C14	112.1 (2)	O2—C7—C6	124.1 (3)
C5—C1—C11	106.6 (2)	O2—C7—C8	125.7 (3)
C5—C1—C14	118.6 (2)	C6—C7—C8	110.2 (2)
C11—C1—C14	105.0 (2)	C7—C8—C9	104.7 (3)
O1—C2—O1	124.1 (3)	C5—C9—C8	106.4 (3)
O1—C2—C3	124.8 (3)	C5—C9—C10	102.6 (2)
C1—C2—C3	111.1 (2)	C8—C9—C10	115.3 (3)
C2—C3—C4	104.1 (2)	C9—C10—C11	104.3 (2)
C3—C4—C5	105.3 (3)	C1—C11—C10	104.4 (2)
C1—C5—C4	105.9 (2)	C1—C11—C12	105.5 (2)
C1—C5—C6	118.7 (2)	C10—C11—C12	115.4 (2)
C1—C5—C9	104.0 (2)	C11—C12—C13	104.3 (3)
C4—C5—C6	111.7 (3)	C12—C13—C14	103.2 (2)
C4—C5—C9	113.0 (2)	C1—C14—C13	105.5 (2)

(III)

C2—O2—C9	113.1 (2)	C4—C8—C7	103.5 (2)
C2—C1—C11	114.4 (2)	C4—C8—C9	114.5 (2)
C2—C1—C14	114.0 (2)	C7—C8—C9	116.1 (2)
C11—C1—C14	103.1 (2)	O2—C9—C8	110.1 (2)
O1—C2—O2	105.6 (2)	O2—C9—C10	108.0 (2)
O1—C2—C1	106.3 (2)	O2—C9—C15	104.1 (2)
O1—C2—C3	110.2 (2)	C8—C9—C10	113.1 (2)
O2—C2—C1	110.2 (2)	C8—C9—C15	112.1 (2)
O2—C2—C3	107.8 (2)	C10—C9—C15	109.0 (2)
C1—C2—C3	116.2 (2)	C9—C10—C11	115.5 (2)
C2—C3—C4	114.6 (2)	C1—C11—C10	110.2 (2)
C3—C4—C5	112.0 (2)	C1—C11—C12	103.5 (2)
C3—C4—C8	110.8 (2)	C10—C11—C12	111.6 (2)
C5—C5—C8	103.9 (2)	C11—C12—C13	106.3 (3)
C4—C5—C6	106.4 (3)	C12—C13—C14	107.6 (3)
C5—C6—C7	109.0 (3)	C1—C14—C13	105.5 (2)
C6—C7—C8	106.0 (3)		

The programs used were *UNICS*III (Sakurai & Kobayashi, 1979) and *ORTEP* (Johnson, 1965). Calculations were performed on a FACOM M780/10 computer at Keio University.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55532 (20 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS1019]

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Structure of a 6-(Tetrahydroxybutyl)-Substituted Pteridine

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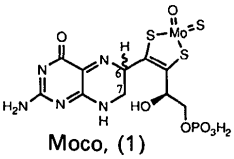
Abstract

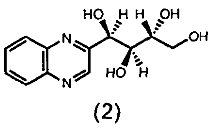
The structure of 2-acetamido-3,4-dihydro-4-oxo-6-(D-*arabino*-tetrahydroxybutyl)pteridine tetraacetate shows that reaction of 2,5,6-triaminopyrimidin-4-one with 1-*p*-toluidino-1-deoxyfructose can be utilized for a convenient method of preparing pteridines carrying a functionalized C_4 side chain at C6.

Comment

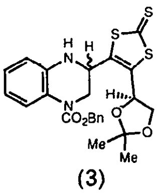
We are developing a synthetic route (Rowe, Garner & Joule, 1985; Larsen, Garner & Joule, 1989; Larsen, Rowe, Garner & Joule, 1989; Russell, Garner & Joule, 1992*a*,*b*) to Moco (Rajagopalan, 1991; Johnson, 1980; Gardlik & Rajagopalan, 1990) (1), the cofactor of all molybdoenzymes except nitrogenase. The cofactor is composed of a dihydropteridine carrying a functionalized side chain at C6 on which are situated the S atoms that coordinate the metal centre; any synthetic plan therefore requires an unambiguous route to a pteridine carrying a heavily functionalized C_4 side chain at C6. In model work, (tetrahydroxybutyl)quinoxaline (2) proved to be a very convenient, easily accessed and useful intermediate; we were able, for example, to transform it into (3). It was obvious that we should attempt to extrapolate this principle and look to the use of an analogous pteridine, (4*a*).



Moco, (1)



(2)



(3)