X-Ray structure determination of 6-epi-brianthein Y (**1**). *Crystal Data:* empirical formula: $C_{28}H_{37}ClO_{10}$; formula weight: 570.5 amu; crystal color and habit: colorless cube roughly 0.4 mm on an edge; orthorhombic space group $P2_12_12_1$; Z = 4; Unit cell dimensions from 25 reflections ($25° \leq 2\theta \leq 40°$) a = 10.381(3), b = 13.830(3), c = 20.132(5) Å; Volume = 2890(1) $Å^3$; $\rho_{calc.}$ = 1.294 gm/cc. *Data collection:* CuK$\bar{\alpha}$ radiation; $2\theta \leq 114°$; variable speed θ:2θ scans; 3941 unique reflections; room temperature. *Solution and refinement:* direct methods (SHELXTL); full-matrix least-squares on F^2; anisotropic nonhydrogens and isotropic riding hydrogens (352 parameters); R = 0.058 for all data. Archival X-ray data have been deposited with the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, U.K.

Table 1. Crystal data and structure refinement for 6-epi-brianthern Y

Identification code	6-epi-brianthern Y
Empirical formula	$C_{28}H_{37}ClO_{10}$
Formula weight	570.5
Temperature	293(2) K
Wavelength	1.54000 Å
Crystal system	Orthorhombic
Space group	P212121
Unit cell dimensions	a = 10.381(3) Å α = 90.00(3)°
	b = 13.830(3) Å β = 90.00(3)°
	c = 20.132(5) Å γ = 90.00(3)°
Volume	2890.4(13) $Å^3$
Z	4
Density (calculated)	1.294 Mg/m^3
Absorption coefficient	1.630 mm^{-1}
F(000)	1196
Crystal size	
θ range for data collection	3.87 to 57.23°
Index ranges	$-11 \le h \le 11$, $0 \le k \le 15$, $0 \le \ell \le 21$
Reflections collected	3941
Independent reflections	3941 (R_{int} = 0.0000)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3941 / 0 / 352
Goodness-of-fit on F^2	1.004
Final R indices [I>2σ(I)]	R1 = 0.0560, wR2 = 0.1474
R indices (all data)	R1 = 0.0583, wR2 = 0.1499
Absolute structure parameter	0.03(3)
Largest diff. peak and hole	0.411 and -0.352 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3]. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cl(1)	1184(2)	313(1)	8534(1)	83(1)
O(1)	4482(3)	631(2)	5609(1)	49(1)
O(2)	5815(4)	1489(2)	6246(2)	81(1)
O(3)	85(3)	-3274(3)	8612(2)	75(1)
O(4)	764(3)	-1798(2)	8348(1)	56(1)
O(5)	470(3)	-2457(2)	5813(2)	68(1)
O(6)	3353(2)	-2297(2)	7774(1)	52(1)
O(7)	1474(2)	-1342(2)	6447(1)	40(1)
O(8)	6215(3)	-2132(2)	7189(2)	59(1)
O(9)	8363(3)	-2134(3)	7072(2)	83(1)
O(10)	6508(3)	-826(2)	6154(2)	61(1)
C(1)	4117(4)	-1032(3)	5919(2)	40(1)
C(2)	4097(4)	31(3)	6181(2)	42(1)
C(3)	2849(4)	449(3)	6438(2)	46(1)
C(4)	2467(4)	468(3)	7065(2)	48(1)
C(5)	3105(4)	42(3)	7648(2)	46(1)
C(6)	2256(4)	-534(3)	8116(2)	54(1)
C(7)	1436(4)	-1318(3)	7800(2)	44(1)
C(8)	2161(3)	-2151(3)	7449(2)	40(1)
C(9)	2428(3)	-2021(3)	6686(2)	37(1)
C(10)	3842(3)	-1739(2)	6518(2)	37(1)
C(11)	4583(4)	-2707(3)	6463(2)	46(1)
C(12)	6030(4)	-2516(3)	6522(2)	53(1)
C(13)	6453(4)	-1835(3)	5988(2)	58(1)
C(14)	5520(4)	-1167(3)	5690(2)	53(1)
C(15)	3257(4)	-1158(3)	5300(2)	53(1)
C(16)	4349(4)	151(3)	7799(2)	58(1)
C(17)	1220(4)	-2997(3)	7566(2)	47(1)
C(18)	1753(5)	-4015(3)	7522(3)	63(1)
C(19)	627(4)	-2747(3)	8224(2)	55(1)
C(20)	4341(5)	-3297(3)	5833(2)	63(1)
C(21)	5397(5)	1304(3)	5710(2)	59(1)
C(22)	5809(7)	1752(4)	5062(3)	93(2)
C(23)	6635(10)	2611(9)	5125(4)	168(5)
C(24)	5806(17)	3497(7)	5324(5)	153(7)
C(25)	541(4)	-1644(3)	6022(2)	47(1)
C(26)	-323(4)	-812(4)	5865(2)	60(1)
C(27)	7427(4)	-1984(3)	7404(3)	63(1)
C(28)	7419(5)	-1634(5)	8100(3)	81(2)

Table 3. Bond lengths [Å] and angles [°].

Cl(1)-C(6)	1.823(4)	O(1)-C(21)	1.346(5)
O(1)-C(2)	1.474(4)	O(2)-C(21)	1.190(5)
O(3)-C(19)	1.207(5)	O(4)-C(19)	1.344(6)
O(4)-C(7)	1.464(5)	O(5)-C(25)	1.202(5)
O(6)-C(8)	1.415(4)	O(7)-C(25)	1.358(5)
O(7)-C(9)	1.447(4)	O(8)-C(27)	1.346(5)
O(8)-C(12)	1.455(5)	O(9)-C(27)	1.197(6)
O(10)-C(13)	1.437(5)	O(10)-C(14)	1.465(5)
C(1)-C(14)	1.539(6)	C(1)-C(15)	1.543(5)
C(1)-C(2)	1.562(5)	C(1)-C(10)	1.579(5)
C(2)-C(3)	1.510(6)	C(3)-C(4)	1.324(6)
C(4)-C(5)	1.470(6)	C(5)-C(16)	1.336(6)
C(5)-C(6)	1.517(6)	C(6)-C(7)	1.518(6)
C(7)-C(8)	1.547(5)	C(8)-C(17)	1.542(5)
C(8)-C(9)	1.573(5)	C(9)-C(10)	1.556(5)
C(10)-C(11)	1.548(5)	C(11)-C(20)	1.528(6)
C(11)-C(12)	1.530(6)	C(12)-C(13)	1.496(6)
C(13)-C(14)	1.466(6)	C(17)-C(19)	1.500(6)
C(17)-C(18)	1.516(6)	C(21)-C(22)	1.506(7)
C(22)-C(23)	1.471(10)	C(23)-C(24)	1.55(2)
C(25)-C(26)	1.493(6)	C(27)-C(28)	1.482(8)

C(21)-O(1)-C(2)	117.6(3)	C(19)-O(4)-C(7)	110.7(3)
C(25)-O(7)-C(9)	119.8(3)	C(27)-O(8)-C(12)	118.4(3)
C(13)-O(10)-C(14)	60.7(3)	C(14)-C(1)-C(15)	107.0(3)
C(14)-C(1)-C(2)	103.2(3)	C(15)-C(1)-C(2)	111.8(3)
C(14)-C(1)-C(10)	109.0(3)	C(15)-C(1)-C(10)	116.2(3)
C(2)-C(1)-C(10)	108.8(3)	O(1)-C(2)-C(3)	106.6(3)
O(1)-C(2)-C(1)	105.2(3)	C(3)-C(2)-C(1)	119.1(3)
C(4)-C(3)-C(2)	126.2(4)	C(3)-C(4)-C(5)	128.2(4)
C(16)-C(5)-C(4)	124.9(4)	C(16)-C(5)-C(6)	118.7(4)
C(4)-C(5)-C(6)	116.4(4)	C(5)-C(6)-C(7)	116.1(3)
C(5)-C(6)-Cl(1)	107.7(3)	C(7)-C(6)-Cl(1)	108.0(3)
O(4)-C(7)-C(6)	106.0(3)	O(4)-C(7)-C(8)	103.7(3)
C(6)-C(7)-C(8)	116.7(3)	O(6)-C(8)-C(17)	112.1(3)
O(6)-C(8)-C(7)	108.7(3)	C(17)-C(8)-C(7)	100.8(3)
O(6)-C(8)-C(9)	108.3(3)	C(17)-C(8)-C(9)	110.3(3)
C(7)-C(8)-C(9)	116.6(3)	O(7)-C(9)-C(10)	114.2(3)
O(7)-C(9)-C(8)	106.1(3)	C(10)-C(9)-C(8)	114.0(3)
C(11)-C(10)-C(9)	105.5(3)	C(11)-C(10)-C(1)	113.0(3)
C(9)-C(10)-C(1)	119.5(3)	C(20)-C(11)-C(12)	108.6(3)
C(20)-C(11)-C(10)	116.1(3)	C(12)-C(11)-C(10)	109.4(3)
O(8)-C(12)-C(13)	113.3(3)	O(8)-C(12)-C(11)	105.4(3)
C(13)-C(12)-C(11)	109.9(4)	O(10)-C(13)-C(14)	60.6(3)
O(10)-C(13)-C(12)	117.0(4)	C(14)-C(13)-C(12)	119.8(3)
O(10)-C(14)-C(13)	58.7(3)	O(10)-C(14)-C(1)	115.6(3)
C(13)-C(14)-C(1)	125.4(3)	C(19)-C(17)-C(18)	114.5(3)
C(19)-C(17)-C(8)	102.7(3)	C(18)-C(17)-C(8)	117.7(3)
O(3)-C(19)-O(4)	121.2(4)	O(3)-C(19)-C(17)	128.6(4)

O(4)-C(19)-C(17)	110.2(3)	O(2)-C(21)-O(1)	122.9(4)
O(2)-C(21)-C(22)	126.4(4)	O(1)-C(21)-C(22)	110.7(4)
C(23)-C(22)-C(21)	115.0(5)	C(22)-C(23)-C(24)	109.7(9)
O(5)-C(25)-O(7)	123.5(4)	O(5)-C(25)-C(26)	127.6(4)
O(7)-C(25)-C(26)	109.0(4)	O(9)-C(27)-O(8)	123.6(5)
O(9)-C(27)-C(28)	126.0(5)	O(8)-C(27)-C(28)	110.4(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3].

The anisotropic displacement factor exponent takes the form:

$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Cl(1)	104(1)	84(1)	60(1)	-27(1)	23(1)	-6(1)
O(1)	65(2)	44(1)	38(1)	8(1)	-5(1)	-10(1)
O(2)	115(3)	67(2)	61(2)	-2(2)	-18(2)	-39(2)
O(3)	81(2)	86(2)	60(2)	14(2)	20(2)	-23(2)
O(4)	59(2)	69(2)	41(1)	2(1)	9(1)	-7(2)
O(5)	77(2)	65(2)	63(2)	-10(2)	-25(2)	-8(2)
O(6)	42(1)	68(2)	47(2)	19(1)	-10(1)	-7(1)
O(7)	43(1)	43(1)	34(1)	0(1)	-8(1)	0(1)
O(8)	43(1)	75(2)	60(2)	4(2)	2(1)	10(1)
O(9)	44(2)	115(3)	89(3)	16(2)	7(2)	14(2)
O(10)	46(2)	52(2)	85(2)	2(2)	3(2)	-3(1)
C(1)	48(2)	38(2)	35(2)	3(2)	4(2)	-2(2)
C(2)	53(2)	39(2)	34(2)	5(2)	-2(2)	-6(2)
C(3)	56(2)	34(2)	49(2)	2(2)	-7(2)	2(2)
C(4)	55(2)	39(2)	51(2)	-4(2)	2(2)	2(2)
C(5)	57(2)	39(2)	41(2)	-14(2)	1(2)	-3(2)
C(6)	67(3)	58(2)	37(2)	-7(2)	-1(2)	-5(2)
C(7)	49(2)	55(2)	29(2)	1(2)	2(2)	-3(2)
C(8)	38(2)	45(2)	37(2)	4(2)	-3(2)	-2(2)
C(9)	39(2)	39(2)	34(2)	1(1)	-5(1)	1(2)
C(10)	44(2)	36(2)	32(2)	2(1)	0(2)	0(2)
C(11)	53(2)	39(2)	45(2)	1(2)	10(2)	5(2)
C(12)	51(2)	49(2)	58(2)	3(2)	10(2)	11(2)
C(13)	51(2)	53(2)	69(3)	1(2)	20(2)	8(2)
C(14)	60(2)	49(2)	48(2)	2(2)	14(2)	0(2)
C(15)	67(3)	59(2)	33(2)	0(2)	0(2)	-10(2)
C(16)	70(3)	60(3)	45(2)	-13(2)	-10(2)	-11(2)
C(17)	43(2)	50(2)	47(2)	9(2)	-2(2)	-5(2)
C(18)	64(3)	53(2)	73(3)	12(2)	4(2)	-7(2)
C(19)	48(2)	71(3)	46(2)	6(2)	-1(2)	-10(2)
C(20)	83(3)	44(2)	60(3)	-8(2)	9(2)	5(2)
C(21)	82(3)	44(2)	51(3)	2(2)	-9(2)	-18(2)
C(22)	138(6)	76(3)	64(3)	19(3)	3(3)	-44(4)
C(23)	178(9)	250(12)	77(5)	67(7)	-29(5)	-130(9)
C(24)	330(23)	58(5)	71(6)	-4(5)	-50(10)	-25(9)
C(25)	49(2)	59(3)	32(2)	0(2)	-5(2)	-8(2)
C(26)	53(2)	74(3)	51(2)	3(2)	-12(2)	7(2)
C(27)	47(2)	65(3)	76(3)	16(2)	-4(2)	7(2)
C(28)	64(3)	101(4)	79(4)	7(3)	-14(3)	2(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3).

	x	y	z	U(eq)
H(6A)	3272(2)	-2742(2)	8062(1)	80
H(2A)	4739(4)	94(3)	6521(2)	80
H(3A)	2276(4)	726(3)	6116(2)	80
H(4A)	1673(4)	801(3)	7149(2)	80
H(6B)	2800(4)	-829(3)	8445(2)	80
H(7A)	822(4)	-1034(3)	7501(2)	80
H(9A)	2259(3)	-2631(3)	6475(2)	80
H(10A)	4172(3)	-1421(2)	6906(2)	80
H(11A)	4333(4)	-3100(3)	6834(2)	80
H(12A)	6488(4)	-3115(3)	6480(2)	80
H(13A)	7118(4)	-2068(3)	5698(2)	80
H(14A)	5678(4)	-1011(3)	5233(2)	80
H(15A)	3505(4)	-695(3)	4968(2)	80
H(15B)	3360(4)	-1800(3)	5127(2)	80
H(15C)	2372(4)	-1056(3)	5419(2)	80
H(16A)	4687(4)	-133(3)	8197(2)	80
H(16B)	4906(4)	512(3)	7510(2)	80
H(17A)	553(4)	-2944(3)	7238(2)	80
H(18A)	1073(5)	-4470(3)	7604(3)	80
H(18B)	2103(5)	-4123(3)	7087(3)	80
H(18C)	2418(5)	-4098(3)	7848(3)	80
H(20A)	4843(5)	-3879(3)	5847(2)	80
H(20B)	3443(5)	-3459(3)	5806(2)	80
H(20C)	4582(5)	-2923(3)	5451(2)	80
H(22A)	5052(7)	1913(4)	4812(3)	80
H(22B)	6282(7)	1278(4)	4813(3)	80
H(23A)	7068(10)	2737(9)	4713(4)	80
H(23B)	7279(10)	2503(9)	5459(4)	80
H(24A)	6354(17)	4052(7)	5365(5)	80
H(24B)	5171(17)	3613(7)	4987(5)	80
H(24C)	5383(17)	3377(7)	5741(5)	80
H(26A)	-986(4)	-1017(4)	5564(2)	80
H(26B)	-708(4)	-579(4)	6268(2)	80
H(26C)	169(4)	-302(4)	5663(2)	80
H(28A)	8289(5)	-1532(5)	8247(3)	80
H(28B)	6953(5)	-1035(5)	8123(3)	80
H(28C)	7011(5)	-2105(5)	8379(3)	80