

C(6)	5622(6)	4997(9)	-1614(4)	60(2)
O(2)	6331(4)	5121(5)	-869(3)	58(1)
C(7)	7016(6)	3425(7)	1580(5)	56(2)
O(6)	6461(4)	2371(5)	1277(4)	68(2)
C(8)	8217(6)	3180(9)	1798(6)	73(2)
O(7)	8687(5)	4195(7)	2234(3)	91(2)
Si(1)	9907(4)	4608(8)	2595(4)	99(2)
C(9)	10011(18)	6269(11)	2426(13)	221(17)
C(10)	10909(9)	3752(23)	2068(10)	185(11)
C(11)	10045(8)	4268(12)	3705(5)	139(5)
C(12)	11215(9)	4186(17)	4089(7)	160(5)
C(13)	11929(14)	5235(24)	3892(14)	170(7)
C(14)	11289(17)	3943(28)	5009(9)	176(8)
C(15)	9422(17)	5271(19)	4142(8)	217(14)
C(16)	9440(15)	3043(16)	3837(10)	159(6)
Si(1B)	9969(8)	4617(16)	2435(9)	99(2)
C(9B)	10071(29)	6143(27)	1973(21)	226(18)
C(10B)	10819(13)	3488(39)	1976(20)	184(12)
C(11B)	10280(17)	4691(21)	3555(10)	146(5)
C(12B)	10389(24)	3500(24)	3990(14)	153(5)
C(13B)	10183(42)	2395(23)	3473(23)	159(6)
C(14B)	11420(36)	3409(38)	4600(25)	172(7)
C(15B)	11380(26)	5430(33)	3754(18)	165(7)
C(16B)	9365(32)	5471(39)	3907(16)	218(14)
Si(2)	4665(1)	5014(3)	1548(1)	48(1)
C(17)	3464(6)	5957(8)	1168(5)	61(2)
C(18)	4175(6)	3481(8)	1826(5)	65(2)
C(19)	5352(5)	5784(6)	2488(3)	68(2)
C(20)	6321(5)	6441(6)	2493(4)	78(3)
C(21)	6763(6)	7024(7)	3201(5)	116(4)
C(22)	6237(8)	6951(9)	3904(4)	128(5)
C(23)	5268(9)	6294(9)	3899(3)	151(7)
C(24)	4826(6)	5710(8)	3190(4)	116(4)
O(3)	3404(3)	3768(5)	-442(3)	51(1)
C(25)	2393(5)	4204(7)	-648(4)	51(2)
O(4)	2190(4)	5182(6)	-969(4)	72(2)

C(26)	1542(3)	3340(4)	-451(3)	47(2)
C(27)	1818(3)	2235(4)	-79(3)	60(2)
C(28)	998(4)	1466(4)	136(4)	72(2)
C(29)	-98(3)	1803(5)	-23(4)	77(3)
C(30)	-374(2)	2908(5)	-395(4)	69(2)
C(31)	446(3)	3677(4)	-609(3)	59(2)
O(5)	6111(5)	4309(6)	-2201(3)	70(2)
C(32)	6974(7)	4893(11)	-2558(4)	75(2)
C(33)	6655(8)	4936(11)	-3492(4)	88(3)
C(34)	7675(12)	5378(17)	-3882(8)	135(6)
C(35)	8622(14)	4561(23)	-3667(10)	185(10)
C(36)	8979(11)	4612(19)	-2729(9)	145(6)
C(37)	7985(10)	4121(14)	-2341(7)	118(5)
C(38)	5655(6)	5724(8)	-3696(4)	85(3)
C(39)	5714(8)	6955(8)	-3865(4)	104(3)
C(40)	4756(12)	7627(9)	-4037(5)	143(6)
C(41)	3739(9)	7067(16)	-4038(7)	196(12)
C(42)	3680(6)	5836(16)	-3869(7)	209(13)
C(43)	4638(9)	5164(10)	-3698(5)	130(5)

Table 8. Bond lengths (Å) for alcohol (-)-27a.

Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
N-O(1)	1.388(7)	N-O(2)	1.468(8)	N-C(3)	1.474(9)
O(1)-C(1)	1.472(8)	C(1)-C(7)	1.530(10)	C(1)-C(2)	1.536(9)
C(2)-C(3)	1.521(10)	C(2)-Si(2)	1.901(6)	C(3)-C(4)	1.505(9)
C(4)-O(3)	1.450(8)	C(4)-C(5)	1.545(10)	C(5)-C(6)	1.524(11)
C(6)-O(5)	1.414(10)	C(6)-O(2)	1.430(9)	C(7)-O(6)	1.411(9)
C(7)-C(8)	1.500(11)	C(8)-O(7)	1.418(11)	O(7)-Si(1)	1.612(7)
O(7)-Si(1B)	1.636(9)	Si(1)-C(10)	1.841(8)	Si(1)-C(11)	1.858(7)
Si(1)-C(9)	1.859(7)	C(11)-C(12)	1.505(8)	C(11)-C(15)	1.564(9)
C(11)-C(16)	1.568(9)	C(12)-C(13)	1.508(10)	C(12)-C(14)	1.532(9)
Si(1B)-C(10B)	1.838(11)	Si(1B)-C(11B)	1.847(10)	Si(1B)-C(9B)	1.858(11)
C(11B)-C(12B)	1.496(12)	C(11B)-C(16B)	1.574(13)	C(11B)-C(15B)	1.578(12)

C(12B)-C(13B)	1.493(14)	C(12B)-C(14B)	1.528(14)	Si(2)-C(17)	1.854(8)
Si(2)-C(18)	1.868(8)	Si(2)-C(19)	1.882(4)	C(19)-C(20)	1.39
C(19)-C(24)	1.39	C(20)-C(21)	1.39	C(21)-C(22)	1.39
C(22)-C(23)	1.39	C(23)-C(24)	1.39	O(3)-C(25)	1.337(8)
C(25)-O(4)	1.215(9)	C(25)-C(26)	1.475(8)	C(26)-C(27)	1.39
C(26)-C(31)	1.39	C(27)-C(28)	1.39	C(28)-C(29)	1.39
C(29)-C(30)	1.39	C(30)-C(31)	1.39	O(5)-C(32)	1.420(11)
C(32)-C(37)	1.514(14)	C(32)-C(33)	1.547(10)	C(33)-C(38)	1.510(12)
C(33)-C(34)	1.55(2)	C(34)-C(35)	1.48(2)	C(35)-C(36)	1.56(2)
C(36)-C(37)	1.53(2)	C(38)-C(39)	1.39	C(38)-C(43)	1.39
C(39)-C(40)	1.39	C(40)-C(41)	1.39	C(41)-C(42)	1.39
		C(42)-C(43)	1.39		

Table 9. Bond angles (deg) for alcohol (-)-27a.

Bond angle	Angle (°)	Bond angle	Angle (°)
O(1)-N-O(2)	103.4(5)	O(1)-N-C(3)	106.2(5)
O(2)-N-C(3)	104.8(5)	N-O(1)-C(1)	110.6(4)
O(1)-C(1)-C(7)	108.7(6)	O(1)-C(1)-C(2)	104.1(5)
C(7)-C(1)-C(2)	119.9(6)	C(3)-C(2)-C(1)	99.7(5)
C(3)-C(2)-Si(2)	116.4(4)	C(1)-C(2)-Si(2)	118.9(5)
N-C(3)-C(4)	109.5(5)	N-C(3)-C(2)	104.3(5)
C(4)-C(3)-C(2)	116.7(6)	O(3)-C(4)-C(3)	106.3(5)
O(3)-C(4)-C(5)	108.1(5)	C(3)-C(4)-C(5)	111.8(6)
C(6)-C(5)-C(4)	108.9(6)	O(5)-C(6)-O(2)	112.1(6)
O(5)-C(6)-C(5)	106.1(7)	O(2)-C(6)-C(5)	111.6(6)
C(6)-O(2)-N	106.9(5)	O(6)-C(7)-C(8)	111.0(6)
O(6)-C(7)-C(1)	109.4(5)	C(8)-C(7)-C(1)	112.4(7)
O(7)-C(8)-C(7)	108.2(7)	C(8)-O(7)-Si(1)	135.9(7)
C(8)-O(7)-Si(1B)	130.8(8)	O(7)-Si(1)-C(10)	108.7(5)
O(7)-Si(1)-C(11)	106.6(4)	C(10)-Si(1)-C(11)	111.6(5)
O(7)-Si(1)-C(9)	107.4(5)	C(10)-Si(1)-C(9)	112.0(6)
C(11)-Si(1)-C(9)	110.3(6)	C(12)-C(11)-C(15)	109.8(7)
C(12)-C(11)-C(16)	109.4(7)	C(15)-C(11)-C(16)	106.4(7)
C(12)-C(11)-Si(1)	113.9(6)	C(15)-C(11)-Si(1)	108.4(6)

C(16)-C(11)-Si(1)	108.5(6)	C(11)-C(12)-C(13)	114.3(8)
C(11)-C(12)-C(14)	112.1(8)	C(13)-C(12)-C(14)	112.1(9)
O(7)-Si(1B)-C(10B)	107.4(7)	O(7)-Si(1B)-C(11B)	107.6(6)
C(10B)-Si(1B)-C(11B)	112.2(8)	O(7)-Si(1B)-C(9B)	106.3(7)
C(10B)-Si(1B)-C(9B)	112.2(8)	C(11B)-Si(1B)-C(9B)	110.7(8)
C(12B)-C(11B)-C(16B)	109.4(11)	C(12B)-C(11B)-C(15B)	109.0(10)
C(16B)-C(11B)-C(15B)	105.6(10)	C(12B)-C(11B)-Si(1B)	116.0(8)
C(16B)-C(11B)-Si(1B)	108.5(9)	C(15B)-C(11B)-Si(1B)	107.9(9)
C(13B)-C(12B)-C(11B)	116.3(12)	C(13B)-C(12B)-C(14B)	113.4(14)
C(11B)-C(12B)-C(14B)	113.4(13)	C(17)-Si(2)-C(18)	109.0(4)
C(17)-Si(2)-C(19)	106.9(4)	C(18)-Si(2)-C(19)	109.5(3)
C(17)-Si(2)-C(2)	108.9(3)	C(18)-Si(2)-C(2)	111.6(4)
C(19)-Si(2)-C(2)	110.8(3)	C(20)-C(19)-C(24)	120.0
C(20)-C(19)-Si(2)	123.0(3)	C(24)-C(19)-Si(2)	117.0(3)
C(21)-C(20)-C(19)	120.0	C(20)-C(21)-C(22)	120.0
C(21)-C(22)-C(23)	120.0	C(24)-C(23)-C(22)	120.0
C(23)-C(24)-C(19)	120.0	C(25)-O(3)-C(4)	118.5(6)
O(4)-C(25)-O(3)	124.7(7)	O(4)-C(25)-C(26)	123.7(6)
O(3)-C(25)-C(26)	111.6(6)	C(27)-C(26)-C(31)	120.0
C(27)-C(26)-C(25)	121.4(4)	C(31)-C(26)-C(25)	118.5(4)
C(26)-C(27)-C(28)	120.0	C(27)-C(28)-C(29)	120.0
C(30)-C(29)-C(28)	120.0	C(31)-C(30)-C(29)	120.0
C(30)-C(31)-C(26)	120.0	C(6)-O(5)-C(32)	115.6(7)
O(5)-C(32)-C(37)	105.9(8)	O(5)-C(32)-C(33)	108.0(7)
C(37)-C(32)-C(33)	111.2(8)	C(38)-C(33)-C(34)	113.5(9)
C(38)-C(33)-C(32)	110.4(7)	C(34)-C(33)-C(32)	107.3(9)
C(35)-C(34)-C(33)	110.9(13)	C(34)-C(35)-C(36)	109.9(13)
C(37)-C(36)-C(35)	104.6(13)	C(32)-C(37)-C(36)	111.7(10)
C(39)-C(38)-C(43)	120.0	C(39)-C(38)-C(33)	123.3(8)
C(43)-C(38)-C(33)	116.7(8)	C(40)-C(39)-C(38)	120.0
C(39)-C(40)-C(41)	120.0	C(42)-C(41)-C(40)	120.0
C(43)-C(42)-C(41)	120.0	C(42)-C(43)-C(38)	120.0

Table 10. Dihedral angles [deg] for alcohol (-)-27a.

Dihedral Angle	Angle (°)	Dihedral Angle	Angle (°)
O(2)-N-O(1)-C(1)	98.4(6)	C(3)-N-O(1)-C(1)	-11.6(7)
N-O(1)-C(1)-C(7)	115.7(6)	N-O(1)-C(1)-C(2)	-13.2(7)
O(1)-C(1)-C(2)-C(3)	31.0(7)	C(7)-C(1)-C(2)-C(3)	-90.7(7)
O(1)-C(1)-C(2)-Si(2)	158.6(5)	C(7)-C(1)-C(2)-Si(2)	36.9(9)
O(1)-N-C(3)-C(4)	157.7(5)	O(2)-N-C(3)-C(4)	48.6(6)
O(1)-N-C(3)-C(2)	32.1(7)	O(2)-N-C(3)-C(2)	-77.0(6)
C(1)-C(2)-C(3)-N	-38.3(7)	Si(2)-C(2)-C(3)-N	-167.5(4)
C(1)-C(2)-C(3)-C(4)	-159.3(6)	Si(2)-C(2)-C(3)-C(4)	71.5(7)
N-C(3)-C(4)-O(3)	134.9(5)	C(2)-C(3)-C(4)-O(3)	-106.9(6)
N-C(3)-C(4)-C(5)	17.2(8)	C(2)-C(3)-C(4)-C(5)	135.4(6)
O(3)-C(4)-C(5)-C(6)	-173.0(6)	C(3)-C(4)-C(5)-C(6)	-56.4(9)
C(4)-C(5)-C(6)-O(5)	147.5(6)	C(4)-C(5)-C(6)-O(2)	25.2(10)
O(5)-C(6)-O(2)-N	-78.4(7)	C(5)-C(6)-O(2)-N	40.4(8)
O(1)-N-O(2)-C(6)	165.7(5)	C(3)-N-O(2)-C(6)	-83.2(6)
O(1)-C(1)-C(7)-O(6)	-56.9(7)	C(2)-C(1)-C(7)-O(6)	62.5(8)
O(1)-C(1)-C(7)-C(8)	66.9(7)	C(2)-C(1)-C(7)-C(8)	-173.7(6)
O(6)-C(7)-C(8)-O(7)	-169.4(7)	C(1)-C(7)-C(8)-O(7)	67.7(9)
C(7)-C(8)-O(7)-Si(1)	-174.8(7)	C(7)-C(8)-O(7)-Si(1B)	-163.0(9)
C(8)-O(7)-Si(1)-C(10)	19.9(12)	Si(1B)-O(7)-Si(1)-C(10)	-44(6)
C(8)-O(7)-Si(1)-C(11)	-100.6(10)	Si(1B)-O(7)-Si(1)-C(11)	-164(6)
C(8)-O(7)-Si(1)-C(9)	141.3(11)	Si(1B)-O(7)-Si(1)-C(9)	78(6)
O(7)-Si(1)-C(11)-C(12)	160.1(9)	C(10)-Si(1)-C(11)-C(12)	41.6(11)
C(9)-Si(1)-C(11)-C(12)	-83.6(11)	O(7)-Si(1)-C(11)-C(15)	-77.3(10)
C(10)-Si(1)-C(11)-C(15)	164.2(12)	C(9)-Si(1)-C(11)-C(15)	39.0(12)
O(7)-Si(1)-C(11)-C(16)	37.9(10)	C(10)-Si(1)-C(11)-C(16)	-80.6(11)
C(9)-Si(1)-C(11)-C(16)	154.2(11)	C(15)-C(11)-C(12)-C(13)	-72(2)
C(16)-C(11)-C(12)-C(13)	171(2)	Si(1)-C(11)-C(12)-C(13)	49(2)
C(15)-C(11)-C(12)-C(14)	57(2)	C(16)-C(11)-C(12)-C(14)	-60(2)
Si(1)-C(11)-C(12)-C(14)	178(2)	C(8)-O(7)-Si(1B)-C(10B)	-0.1(14)
Si(1)-O(7)-Si(1B)-C(10B)	125(5)	C(8)-O(7)-Si(1B)-C(11B)	-121.1(11)
Si(1)-O(7)-Si(1B)-C(11B)	4(5)	C(8)-O(7)-Si(1B)-C(9B)	120.3(14)
Si(1)-O(7)-Si(1B)-C(9B)	-115(5)	O(7)-Si(1B)-C(11B)-C(12B)	73(2)

C(10B)-Si(1B)-C(11B)- C(12B)	-45(2)	C(9B)-Si(1B)-C(11B)- C(12B)	-171(2)
O(7)-Si(1B)-C(11B)-C(16B)	-51(2)	C(10B)-Si(1B)-C(11B)- C(16B)	-169(2)
C(9B)-Si(1B)-C(11B)- C(16B)	65(2)	O(7)-Si(1B)-C(11B)-C(15B)	-165(2)
C(10B)-Si(1B)-C(11B)- C(15B)	77(2)	C(9B)-Si(1B)-C(11B)- C(15B)	-49(2)
C(16B)-C(11B)-C(12B)- C(13B)	120(3)	C(15B)-C(11B)-C(12B)- C(13B)	-125(3)
Si(1B)-C(11B)-C(12B)- C(13B)	-3(3)	C(16B)-C(11B)-C(12B)- C(14B)	-106(3)
C(15B)-C(11B)-C(12B)- C(14B)	9(3)	Si(1B)-C(11B)-C(12B)- C(14B)	131(3)
C(3)-C(2)-Si(2)-C(17)	-75.1(6)	C(1)-C(2)-Si(2)-C(17)	165.6(6)
C(3)-C(2)-Si(2)-C(18)	45.3(6)	C(1)-C(2)-Si(2)-C(18)	-74.0(6)
C(3)-C(2)-Si(2)-C(19)	167.6(5)	C(1)-C(2)-Si(2)-C(19)	48.3(7)
C(17)-Si(2)-C(19)-C(20)	-104.2(5)	C(18)-Si(2)-C(19)-C(20)	137.9(5)
C(2)-Si(2)-C(19)-C(20)	14.4(6)	C(17)-Si(2)-C(19)-C(24)	73.5(5)
C(18)-Si(2)-C(19)-C(24)	-44.4(5)	C(2)-Si(2)-C(19)-C(24)	-167.9(4)
C(24)-C(19)-C(20)-C(21)	0.0	Si(2)-C(19)-C(20)-C(21)	177.6(5)
C(19)-C(20)-C(21)-C(22)	0.0	C(20)-C(21)-C(22)-C(23)	0.0
C(21)-C(22)-C(23)-C(24)	0.0	C(22)-C(23)-C(24)-C(19)	0.0
C(20)-C(19)-C(24)-C(23)	0.0	Si(2)-C(19)-C(24)-C(23)	-177.8(5)
C(3)-C(4)-O(3)-C(25)	155.7(5)	C(5)-C(4)-O(3)-C(25)	-84.1(7)
C(4)-O(3)-C(25)-O(4)	2.0(10)	C(4)-O(3)-C(25)-C(26)	-179.0(5)
O(4)-C(25)-C(26)-C(27)	-179.6(6)	O(3)-C(25)-C(26)-C(27)	1.4(7)
O(4)-C(25)-C(26)-C(31)	-2.7(9)	O(3)-C(25)-C(26)-C(31)	178.3(4)
C(31)-C(26)-C(27)-C(28)	0.0	C(25)-C(26)-C(27)-C(28)	176.8(5)
C(26)-C(27)-C(28)-C(29)	0.0	C(27)-C(28)-C(29)-C(30)	0.0
C(28)-C(29)-C(30)-C(31)	0.0	C(29)-C(30)-C(31)-C(26)	0.0
C(27)-C(26)-C(31)-C(30)	0.0	C(25)-C(26)-C(31)-C(30)	-176.9(5)
O(2)-C(6)-O(5)-C(32)	-72.0(9)	C(5)-C(6)-O(5)-C(32)	166.0(6)
C(6)-O(5)-C(32)-C(37)	119.0(9)	C(6)-O(5)-C(32)-C(33)	-121.8(8)
O(5)-C(32)-C(33)-C(38)	65.0(11)	C(37)-C(32)-C(33)-C(38)	-179.2(10)
O(5)-C(32)-C(33)-C(34)	-170.8(10)	C(37)-C(32)-C(33)-C(34)	-55.0(14)

C(38)-C(33)-C(34)-C(35)	-179.3(13)	C(32)-C(33)-C(34)-C(35)	58(2)
C(33)-C(34)-C(35)-C(36)	-65(2)	C(34)-C(35)-C(36)-C(37)	63(2)
O(5)-C(32)-C(37)-C(36)	177.0(11)	C(33)-C(32)-C(37)-C(36)	60(2)
C(35)-C(36)-C(37)-C(32)	-61(2)	C(34)-C(33)-C(38)-C(39)	-28.7(11)
C(32)-C(33)-C(38)-C(39)	91.9(9)	C(34)-C(33)-C(38)-C(43)	152.2(9)
C(32)-C(33)-C(38)-C(43)	-87.2(9)	C(43)-C(38)-C(39)-C(40)	0.0
C(33)-C(38)-C(39)-C(40)	-179.0(7)	C(38)-C(39)-C(40)-C(41)	0.0
C(39)-C(40)-C(41)-C(42)	0.0	C(40)-C(41)-C(42)-C(43)	0.0
C(41)-C(42)-C(43)-C(38)	0.0	C(39)-C(38)-C(43)-C(42)	0.0
C(33)-C(38)-C(43)-C(42)		179.1(6)	

## Crystal Structure of (-)-7-Epiaustraline ((-)-4)

The following was made available by Dr. Scott Wilson, X-ray Crystallographic Laboratory, University of Illinois at Urbana-Champaign.

### Crystal Preparation and Structure Refinement Summary.

Crystals were grown from methanol. The data crystal was mounted using oil (Paratone-N, Exxon) to a thin glass fiber with the (1 0 1) scattering planes roughly normal to the spindle axis. Average intensity beyond 0.9 Å resolution was less than 1 % (I); these data were not used for calculations.

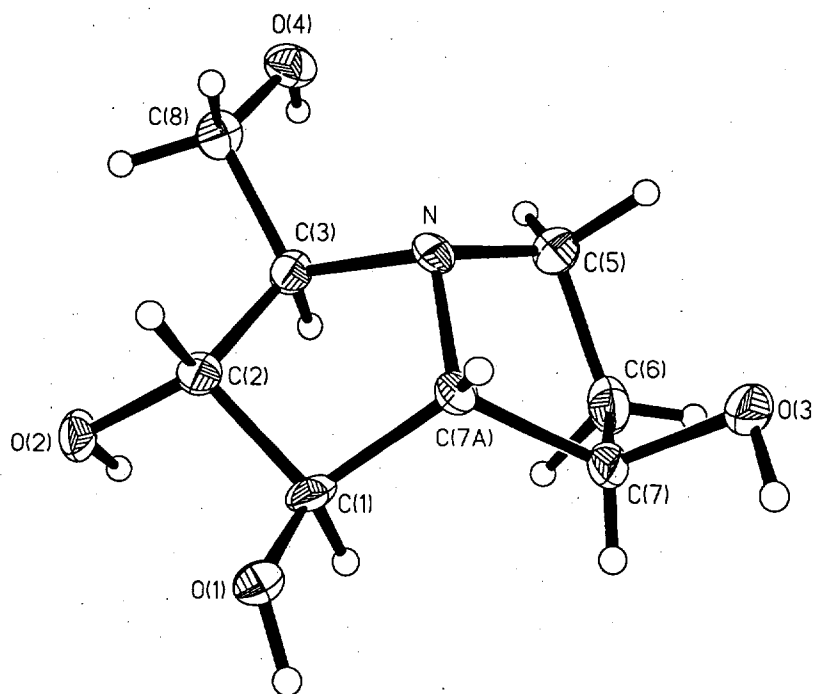
Systematic conditions suggested the unambiguous space group. Structure was solved by direct methods.<sup>8</sup> All positional parameters were independently refined. H atom U's were assigned as 1.2 times U<sub>eq</sub> of adjacent non-H atoms. The space group choice was confirmed by successful convergence of the full-matrix least-squares refinement on F<sup>2</sup>.<sup>9</sup> The highest peaks in the final difference Fourier map were in the vicinity of hydroxyl atoms; the final map had no other significant features. A final analysis of variance between observed and calculated structure factors showed no dependence on amplitude or resolution.

**Table 11.** Crystal Data and Structure Refinement for (-)-7-epiaustraline ((-)-4).

Empirical formula	C <sub>8</sub> H <sub>15</sub> NO <sub>4</sub>	
Formula weight	189.21	
Temperature	198(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 5.0650(8) Å	alpha = 90 deg
from 878 reflns with	b = 8.2073(13) Å	beta = 90 deg
4<=theta<=23	c = 21.408(3) Å	gamma = 90 deg
	V = 889.9(2) Å <sup>3</sup>	Z = 4
Density (calculated)	1.412 Mg/m <sup>3</sup>	
Absorption coefficient	0.113 mm <sup>-1</sup>	



Crystal size	0.07 x 0.11 x 0.22 mm
Theta range for data collection	1.90 to 22.99 deg
Index ranges	-6<=h<=6, -4<=k<=9, -25<=l<=24
Collection method	0.3 deg $\omega$ scans for 0.1667 min/scan
Reflections collected	3837 [R(int) = 0.1884]
Independent reflections	1239 [877 obsI >2sigma(I)]
Absorption correction	None
Refinement (shift/err=0.004)	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	1228 / 0 / 163
Goodness-of-fit on F <sup>2</sup>	1.110
Final R indices (obs data)	R1 = 0.0715, wR2 = 0.1385
R indices (all data)	R1 = 0.1135, wR2 = 0.1615
calc $w=1/[\sigma^2(F_o^2)+(0.0434P)^2+0.0000P]$	
where $P=(F_o^2+2F_c^2)/3$	
Absolute structure parameter	1(4)
Largest diff. peak and hole	0.229 and -0.214 e.Å <sup>-3</sup>



**Figure 3.** SHELXTL<sup>10</sup> plot of 7-epiaustraline ((-)-4) showing 35% probability ellipsoids for non-H atoms and circles of arbitrary size for H atoms.

**Table 12.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{Å}^2 \times 10^3$ ) for (-)-7-epiaustraline ((-)-4).  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor

atom	x	y	z	$U(\text{eq})$
O(1)	-2514(8)	4097(6)	2614(2)	32(1)
O(2)	-5091(7)	6692(5)	1777(2)	33(1)
O(3)	3300(7)	1441(6)	1507(2)	37(1)
O(4)	257(7)	7796(6)	252(2)	36(1)
N	1086(8)	4949(7)	1183(2)	25(1)
C(1)	-2288(11)	4283(8)	1959(3)	26(2)
C(2)	-2477(11)	6052(8)	1758(3)	26(2)
C(3)	-1236(11)	6070(8)	1114(3)	25(2)
C(5)	1593(13)	3956(9)	622(3)	30(2)
C(6)	157(13)	2377(9)	746(3)	35(2)
C(7)	673(11)	2076(9)	1434(3)	32(2)
C(7A)	471(10)	3799(8)	1716(3)	26(2)
C(8)	-550(12)	7753(9)	884(3)	28(2)

**Table 13.** Bond lengths [ $\text{Å}$ ] for (-)-7-epiaustraline ((-)-4).

Bond	Length ( $\text{Å}$ )	Bond	Length ( $\text{Å}$ )	Bond	Length ( $\text{Å}$ )
O(1)-C(1)	1.416(8)	O(1)-H(1A)	0.84(7)	O(2)-C(2)	1.425(7)
O(2)-H(2A)	1.13(7)	O(3)-C(7)	1.438(7)	O(3)-H(3A)	1.03(7)
O(4)-C(8)	1.414(8)	O(4)-H(4A)	0.71(7)	N-C(5)	1.474(8)
N-C(3)	1.501(8)	N-C(7A)	1.514(8)	C(1)-C(2)	1.517(9)
C(1)-C(7A)	1.543(8)	C(1)-H(1)	0.96(6)	C(2)-C(3)	1.513(8)
C(2)-H(2)	1.06(6)	C(3)-C(8)	1.508(10)	C(3)-H(3)	0.97(6)
C(5)-C(6)	1.510(10)	C(5)-H(5A)	1.01(7)	C(5)-H(5B)	1.04(6)
C(6)-C(7)	1.515(10)	C(6)-H(6A)	1.12(6)	C(6)-H(6B)	0.87(7)
C(7)-C(7A)	1.540(9)	C(7)-H(7)	0.84(7)	C(7A)-H(7A)	0.91(6)
C(8)-H(8A)	0.87(6)	C(8)-H(8B)	1.01(6)		

**Table 14.** Bond angles [deg] for (-)-7-epiaustraline ((-)-4).

Bond Angle	Angle (°)	Bond Angle	Angle (°)
C(1)-O(1)-H(1A)	109(5)	C(2)-O(2)-H(2A)	110(3)
C(7)-O(3)-H(3A)	104(4)	C(8)-O(4)-H(4A)	110(6)
C(5)-N-C(3)	113.4(5)	C(5)-N-C(7A)	107.8(5)
C(3)-N-C(7A)	107.1(4)	O(1)-C(1)-C(2)	112.3(6)
O(1)-C(1)-C(7A)	112.3(5)	C(2)-C(1)-C(7A)	102.0(5)
O(1)-C(1)-H(1)	109(4)	C(2)-C(1)-H(1)	117(4)
C(7A)-C(1)-H(1)	103(4)	O(2)-C(2)-C(3)	114.2(5)
O(2)-C(2)-C(1)	113.8(5)	C(3)-C(2)-C(1)	104.0(5)
O(2)-C(2)-H(2)	105(3)	C(3)-C(2)-H(2)	113(3)
C(1)-C(2)-H(2)	107(3)	N-C(3)-C(8)	114.4(5)
N-C(3)-C(2)	103.4(5)	C(8)-C(3)-C(2)	113.7(6)
N-C(3)-H(3)	108(4)	C(8)-C(3)-H(3)	109(4)
C(2)-C(3)-H(3)	107(4)	N-C(5)-C(6)	104.3(5)
N-C(5)-H(5A)	113(4)	C(6)-C(5)-H(5A)	113(3)
N-C(5)-H(5B)	110(3)	C(6)-C(5)-H(5B)	104(4)
H(5A)-C(5)-H(5B)	111(5)	C(5)-C(6)-C(7)	103.2(6)
C(5)-C(6)-H(6A)	116(3)	C(7)-C(6)-H(6A)	110(3)
C(5)-C(6)-H(6B)	116(4)	C(7)-C(6)-H(6B)	110(5)
H(6A)-C(6)-H(6B)	101(5)	O(3)-C(7)-C(6)	108.9(5)
O(3)-C(7)-C(7A)	110.6(5)	C(6)-C(7)-C(7A)	102.7(6)
O(3)-C(7)-H(7)	110(5)	C(6)-C(7)-H(7)	106(4)
C(7A)-C(7)-H(7)	118(5)	N-C(7A)-C(7)	105.3(5)
N-C(7A)-C(1)	106.3(5)	C(7)-C(7A)-C(1)	115.4(5)
N-C(7A)-H(7A)	114(4)	C(7)-C(7A)-H(7A)	103(4)
C(1)-C(7A)-H(7A)	113(4)	O(4)-C(8)-C(3)	113.8(6)
O(4)-C(8)-H(8A)	113(4)	C(3)-C(8)-H(8A)	103(5)
O(4)-C(8)-H(8B)	115(3)	C(3)-C(8)-H(8B)	105(4)
H(8A)-C(8)-H(8B)	107(5)		

**Table 15.** Dihedral angles [deg] for (-)-7-epiaustraline ((-)-4).

Dihedral Angle	Angle (°)	Dihedral Angle	Angle (°)
O(1)-C(1)-C(2)-O(2)	-75.1(7)	C(7A)-C(1)-C(2)-O(2)	164.5(5)
O(1)-C(1)-C(2)-C(3)	160.1(5)	C(7A)-C(1)-C(2)-C(3)	39.7(6)
C(5)-N-C(3)-C(8)	-92.5(6)	C(7A)-N-C(3)-C(8)	148.8(5)
C(5)-N-C(3)-C(2)	143.3(5)	C(7A)-N-C(3)-C(2)	24.6(6)
O(2)-C(2)-C(3)-N	-164.9(5)	C(1)-C(2)-C(3)-N	-40.3(6)
O(2)-C(2)-C(3)-C(8)	70.5(7)	C(1)-C(2)-C(3)-C(8)	-165.0(5)
C(3)-N-C(5)-C(6)	-94.4(6)	C(7A)-N-C(5)-C(6)	24.0(6)
N-C(5)-C(6)-C(7)	-39.5(6)	C(5)-C(6)-C(7)-O(3)	-78.1(6)
C(5)-C(6)-C(7)-C(7A)	39.1(6)	C(5)-N-C(7A)-C(7)	0.5(5)
C(3)-N-C(7A)-C(7)	122.8(5)	C(5)-N-C(7A)-C(1)	-122.4(5)
C(3)-N-C(7A)-C(1)	-0.1(6)	O(3)-C(7)-C(7A)-N	91.6(6)
C(6)-C(7)-C(7A)-N	-24.5(6)	O(3)-C(7)-C(7A)-C(1)	-151.6(6)
C(6)-C(7)-C(7A)-C(1)	92.3(6)	O(1)-C(1)-C(7A)-N	-144.7(5)
C(2)-C(1)-C(7A)-N	-24.3(6)	O(1)-C(1)-C(7A)-C(7)	99.1(7)
C(2)-C(1)-C(7A)-C(7)	-140.5(6)	N-C(3)-C(8)-O(4)	70.0(7)
C(2)-C(3)-C(8)-O(4)	-171.5(5)		

## Australine Data

Table 16. Alexines 1, 8, and 9 and Australines 2-5 and 10.

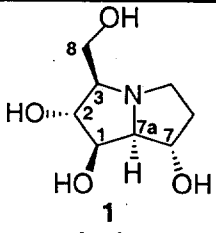
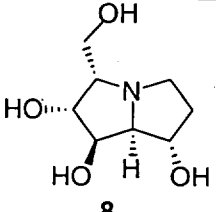
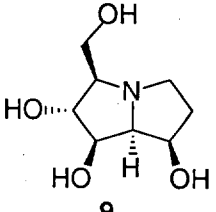
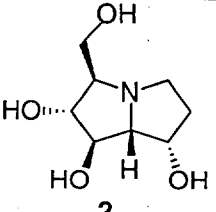
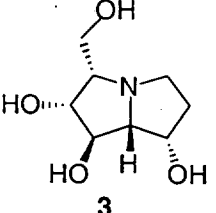
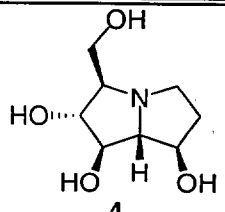
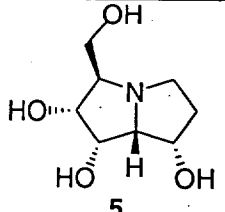
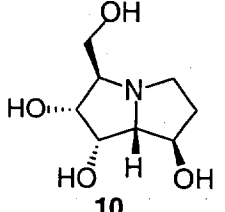
Structure Common Name	CA Name Origin
 <p><b>1</b> <b>alexine</b></p>	<p>(1<i>R</i>,2<i>R</i>,3<i>R</i>,7<i>S</i>,7<i>aS</i>)-hexahydro-3-(hydroxymethyl)-1<i>H</i>-pyrrolizine-1,2,7-triol</p> <p>Natural</p>
 <p><b>8</b> <b>3-epialexine</b></p>	<p>(1<i>R</i>,2<i>R</i>,3<i>S</i>,7<i>S</i>,7<i>aS</i>)-hexahydro-3-(hydroxymethyl)-1<i>H</i>-pyrrolizine-1,2,7-triol</p> <p>Synthetic</p>
 <p><b>9</b> <b>7-epialexine</b></p>	<p>(1<i>R</i>,2<i>R</i>,3<i>R</i>,7<i>R</i>,7<i>aS</i>)-hexahydro-3-(hydroxymethyl)-1<i>H</i>-pyrrolizine-1,2,7-triol</p> <p>Synthetic</p>
 <p><b>2</b> <b>australine</b></p>	<p>(1<i>R</i>,2<i>R</i>,3<i>R</i>,7<i>S</i>,7<i>aR</i>)-hexahydro-3-(hydroxymethyl)-1<i>H</i>-pyrrolizine-1,2,7-triol</p> <p>Natural</p>
 <p><b>3</b> <b>3-epiaustraline</b></p>	<p>(1<i>R</i>,2<i>R</i>,3<i>S</i>,7<i>S</i>,7<i>aR</i>)-hexahydro-3-(hydroxymethyl)-1<i>H</i>-pyrrolizine-1,2,7-triol</p> <p>Natural</p>

Table 16. Alexines 1, 8, and 9 and Australines 2-5 and 10, cont.

Structure Common Name	CA Name Origin
 <p>4 7-epiaustraline</p>	<p>(1<i>R</i>,2<i>R</i>,3<i>R</i>,7<i>R</i>,7<i>aR</i>)-hexahydro-3-(hydroxymethyl)-1<i>H</i>-pyrrolizine-1,2,7-triol</p> <p>Natural</p>
 <p>5 1-epiaustraline</p>	<p>(1<i>S</i>,2<i>R</i>,3<i>R</i>,7<i>S</i>,7<i>aR</i>)-hexahydro-3-(hydroxymethyl)-1<i>H</i>-pyrrolizine-1,2,7-triol</p> <p>Natural</p>
 <p>10 1,7-diepiaustraline</p>	<p>(1<i>S</i>,2<i>R</i>,3<i>S</i>,7<i>R</i>,7<i>aR</i>)-hexahydro-3-(hydroxymethyl)-1<i>H</i>-pyrrolizine-1,2,7-triol</p> <p>Synthetic</p>

**<sup>1</sup>H and <sup>13</sup>C Spectra for (-)-7-Epiaustraline ((-)-4)  
and (-)-1-Epicastanospermine (-)-14).**

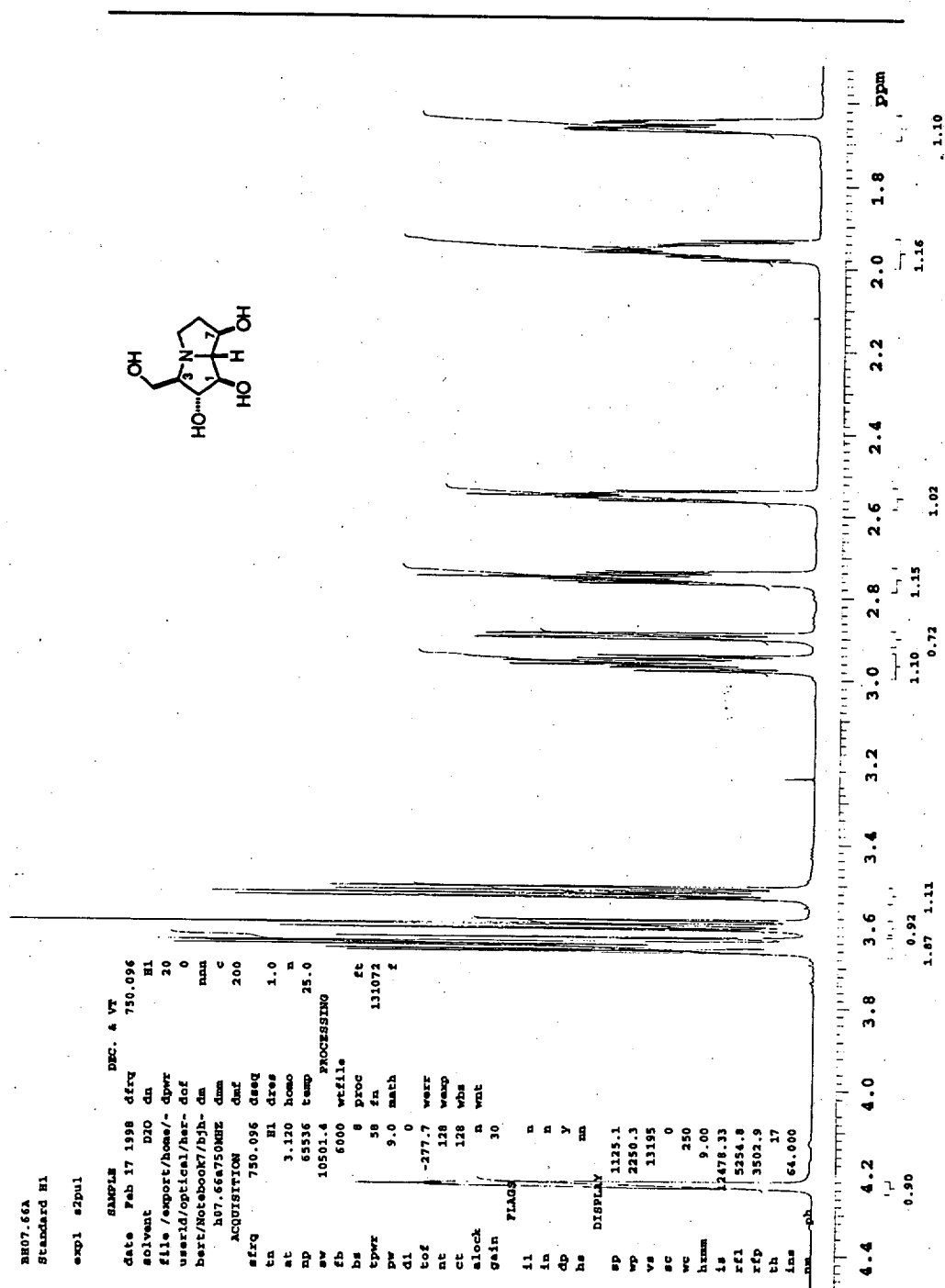
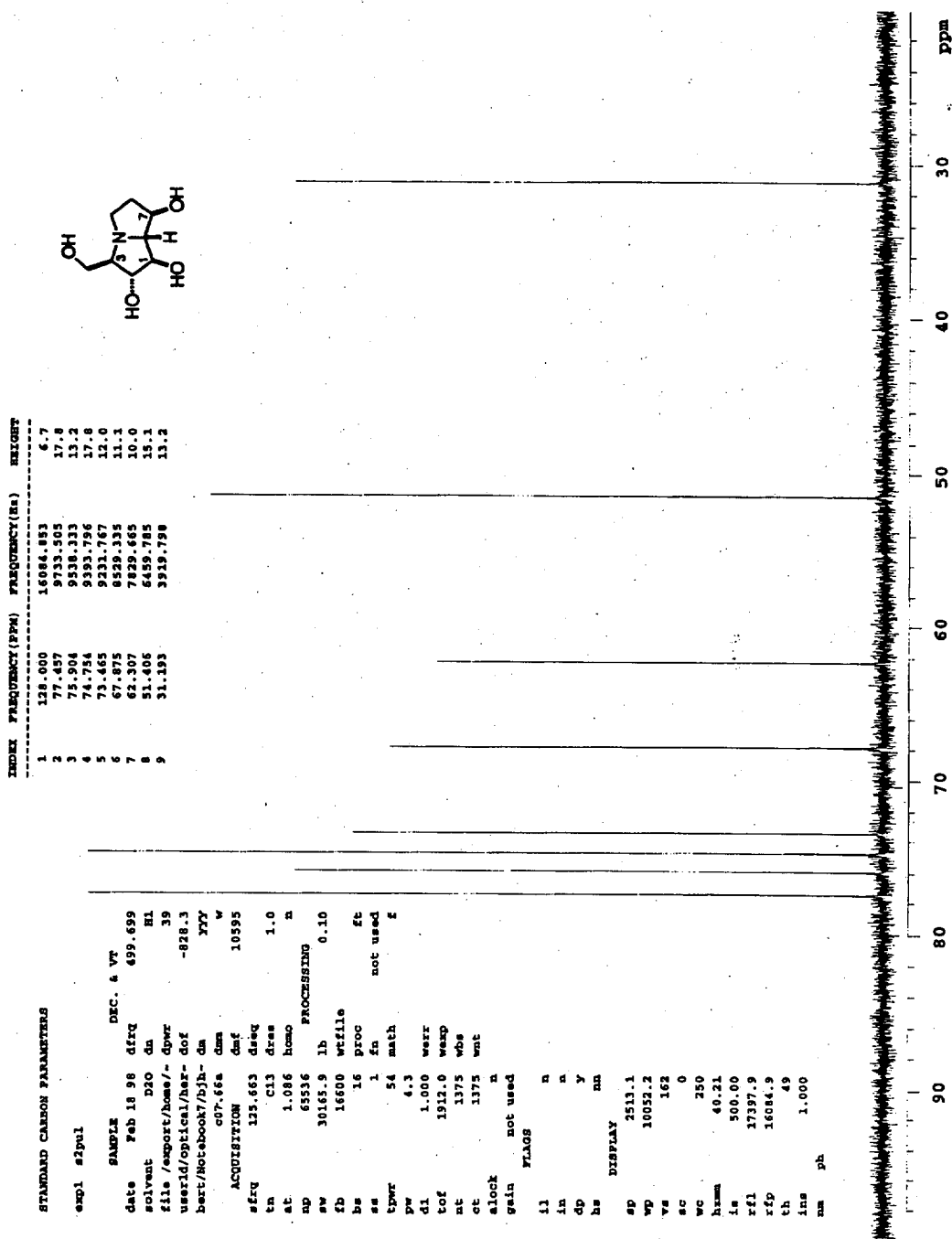


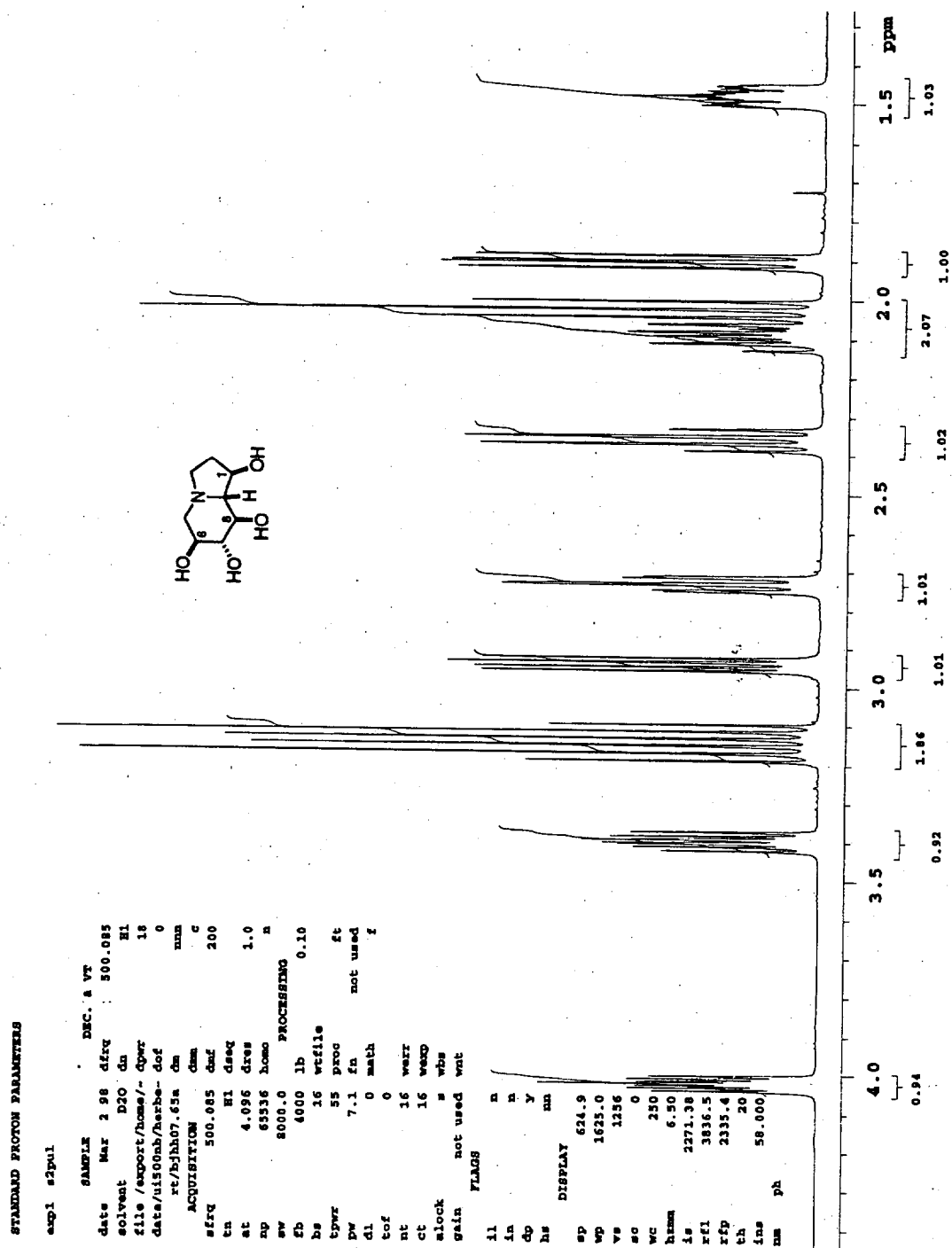
Figure 4. <sup>1</sup>H spectrum (750 MHz) of (-)-7-epiaustraline ((-)-4).

INDEX	FREQUENCY (PPM)	FREQUENCY (Hz)	HEIGHT	INDEX	FREQUENCY (PPM)	FREQUENCY (Hz)	HEIGHT	INDEX	FREQUENCY (PPM)	FREQUENCY (Hz)	HEIGHT
1	4.685	3514.165	207.8	57	4.228	3171.408	941.1	113	1.935	1451.533	201.5
2	4.685	3513.845	217.4	58	3.666	2749.972	1135.2	114	1.674	1255.718	329.9
3	4.684	3513.524	225.5	59	3.663	2746.136	1185.3	115	1.670	1242.673	611.5
4	4.684	3513.204	240.7	60	3.653	2740.197	798.2	116	1.666	1249.789	621.8
5	4.683	3512.883	256.1	61	3.651	2738.274	1550.7	117	1.662	1246.904	616.1
6	4.683	3512.563	269.5	62	3.645	2734.429	1541.3	118	1.657	1242.896	485.8
7	4.682	3512.242	283.4	63	3.641	2732.025	1895.1	119	1.652	1239.233	593.6
8	4.682	3511.922	297.1	64	3.641	2731.384	1421.3	120	1.648	1236.268	587.1
9	4.682	3511.601	312.9	65	3.630	2723.052	1162.1	121	1.644	1233.464	513.4
10	4.681	3511.281	332.0	66	3.610	2707.508	1398.2	122	1.640	1230.400	258.4
11	4.681	3510.960	354.9	67	3.599	2699.496	1945.8				
12	4.680	3510.640	376.8	68	3.588	2691.163	830.6				
13	4.680	3510.319	399.5	69	3.532	2649.661	1405.9				
14	4.679	3509.999	423.0	70	3.524	2643.251	1462.7				
15	4.679	3509.678	450.3	71	3.517	2637.803	1164.7				
16	4.679	3509.358	476.5	72	3.508	2631.553	1177.2				
17	4.678	3509.037	507.2	73	3.508	2635.596	441.5				
18	4.678	3508.717	543.1	74	3.973	2329.988	498.7				
19	4.677	3508.396	583.0	75	2.966	2224.539	748.2				
20	4.677	3508.076	623.8	76	2.958	2218.931	757.2				
21	4.676	3507.755	667.3	77	2.942	2213.963	580.6				
22	4.676	3507.435	715.2	78	2.944	2208.195	530.2				
23	4.676	3507.114	766.3	79	2.902	2176.948	830.2				
24	4.675	3506.794	828.9	80	2.901	2175.666	817.6				
25	4.675	3506.474	884.9	81	2.892	2169.836	802.2				
26	4.674	3506.153	953.1	82	2.770	2077.598	578.8				
27	4.674	3505.833	1026.2	83	2.765	2074.072	639.4				
28	4.673	3505.512	1103.9	84	2.760	2070.387	671.0				
29	4.673	3505.192	1193.7	85	2.753	2066.381	971.9				
30	4.672	3504.871	1290.0	86	2.749	2062.375	561.0				
31	4.672	3504.551	1403.3	87	2.745	2058.689	560.4				
32	4.672	3504.230	1544.2	88	2.740	2055.164	512.8				
33	4.671	3503.910	1708.7	89	2.567	1925.208	530.8				
34	4.671	3503.589	1872.3	90	2.561	1921.202	587.1				
35	4.670	3503.269	2093.8	91	2.558	1918.958	639.1				
36	4.670	3502.948	2324.9	92	2.553	1915.273	854.3				
37	4.669	3502.628	2590.6	93	2.546	1912.228	614.5				
38	4.669	3502.307	2874.8	94	2.546	1909.825	572.2				
39	4.668	3501.987	3207.6	95	2.541	1905.979	489.7				
40	4.668	3501.666	3658.0	96	1.983	1487.427	292.2				
41	4.668	3501.346	4319.8	97	1.976	1482.300	334.3				
42	4.667	3501.025	5126.9	98	1.974	1481.018	343.2				
43	4.665	3499.263	118307.0	99	1.973	1480.216	375.2				
44	4.664	3498.461	11399.6	100	1.970	1477.332	362.3				
45	4.664	3498.141	5334.1	101	1.965	1474.127	577.3				
46	4.663	3497.820	3169.4	102	1.964	1473.005	506.9				
47	4.662	3497.500	2162.6	103	1.961	1471.243	390.4				
48	4.662	3496.859	1129.1	104	1.958	1468.999	537.2				
49	4.658	3494.135	297.2	105	1.956	1467.557	426.8				
50	4.658	3493.814	271.2	106	1.955	1466.596	477.4				
51	4.657	3493.494	243.1	107	1.954	1465.796	509.2				
52	4.657	3493.173	222.6	108	1.952	1464.032	521.7				
53	4.657	3492.853	201.7	109	1.949	1461.628	591.1				
54	4.612	3459.362	298.2	110	1.945	1458.744	388.1				
55	4.234	3176.215	939.5	111	1.943	1457.783	388.1				
56	4.231	3173.972	1112.6	112	1.942	1456.661	363.8				

Figure 5. Peak listing for the  $^1\text{H}$  spectrum (750 MHz) of (-)-7-epiaustraline ((-)-4).



Figure 6.  $^{13}\text{C}$  spectrum (126 MHz) of (-)-7-epiaustraline ((-)-4).

Figure 7.  $^1\text{H}$  spectrum (500 MHz) of (-)-1-epicastanospermine ((-)-14).

INDEX	FREQUENCY (PPM)	FREQUENCY (Hz)	HEIGHT	INDEX	FREQUENCY (PPM)	FREQUENCY (Hz)	HEIGHT
1	4.670	2335.395	8419.1	57	1.475	737.445	183.6
2	4.042	2021.421	219.5	58	1.471	735.493	160.8
3	4.035	2017.758	250.5	59	1.465	732.863	144.2
4	4.029	2014.829	242.7	60	1.461	730.810	138.2
5	4.023	2011.655	276.3	61	1.459	729.901	149.1
6	4.017	2008.725	239.8				
7	4.011	2005.795	282.8				
8	4.004	2002.133	224.5				
9	3.422	1711.352	210.5				
10	3.412	1708.223	247.0				
11	3.405	1702.563	268.3				
12	3.401	1700.854	287.9				
13	3.394	1697.192	315.0				
14	3.390	1695.483	249.4				
15	3.384	1692.065	278.0				
16	3.373	1686.694	250.4				
17	3.189	1594.650	391.2				
18	3.171	1585.616	982.5				
19	3.152	1576.339	756.9				
20	3.134	1567.305	790.4				
21	3.117	1558.216	1013.2				
22	3.098	1548.482	359.8				
23	2.858	1429.412	431.0				
24	2.848	1424.285	459.9				
25	2.837	1418.669	495.7				
26	2.826	1413.298	449.9				
27	2.753	1376.870	211.4				
28	2.749	1374.916	226.4				
29	2.734	1367.104	424.9				
30	2.717	1358.803	265.1				
31	2.714	1357.338	238.2				
32	2.388	1194.247	186.7				
33	2.369	1184.725	435.7				
34	2.351	1175.936	477.4				
35	2.332	1166.414	206.6				
36	2.111	1055.871	234.2				
37	2.101	1050.698	147.5				
38	2.083	1046.337	232.1				
39	2.082	1046.337	232.1				
40	2.064	1041.610	261.7				
41	2.048	1032.377	235.6				
42	2.026	1024.076	539.8				
43	2.003	1013.333	910.2				
44	1.919	959.621	467.9				
45	1.906	953.029	487.4				
46	1.900	950.343	510.5				
47	1.887	943.751	495.2				
48	1.809	784.780	464.0				
49	1.806	783.071	141.6				
50	1.802	781.362	169.8				
51	1.499	749.633	156.6				
52	1.489	746.679	137.2				
53	1.489	744.926	172.4				
54	1.486	743.061	161.9				
55	1.482	741.108	187.6				
56	1.478	739.155	261.2				
			376.8				

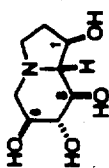
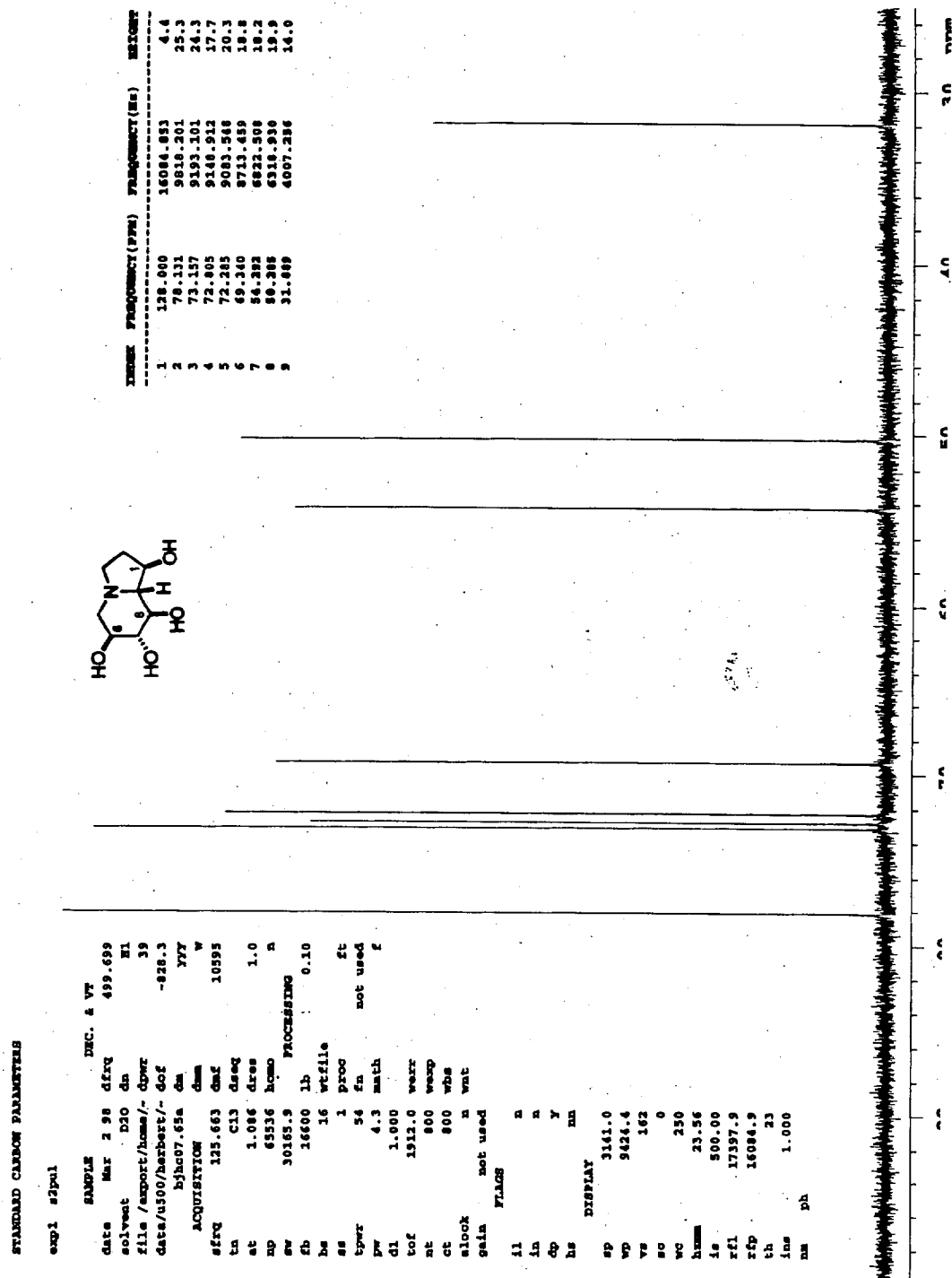


Figure 8. Peak listing for the  $^1\text{H}$  spectrum (500 MHz) of  $(-)$ -1-epicastanospermine  $((-)$ -14).

Figure 9.  $^{13}\text{C}$  spectrum (126 MHz) of (-)-1-epicastanospermine ((-)-14).

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