Supplementary Material for

The Cytosporones, New Octaketide Antibiotics Isolated from an Endophytic Fungus.

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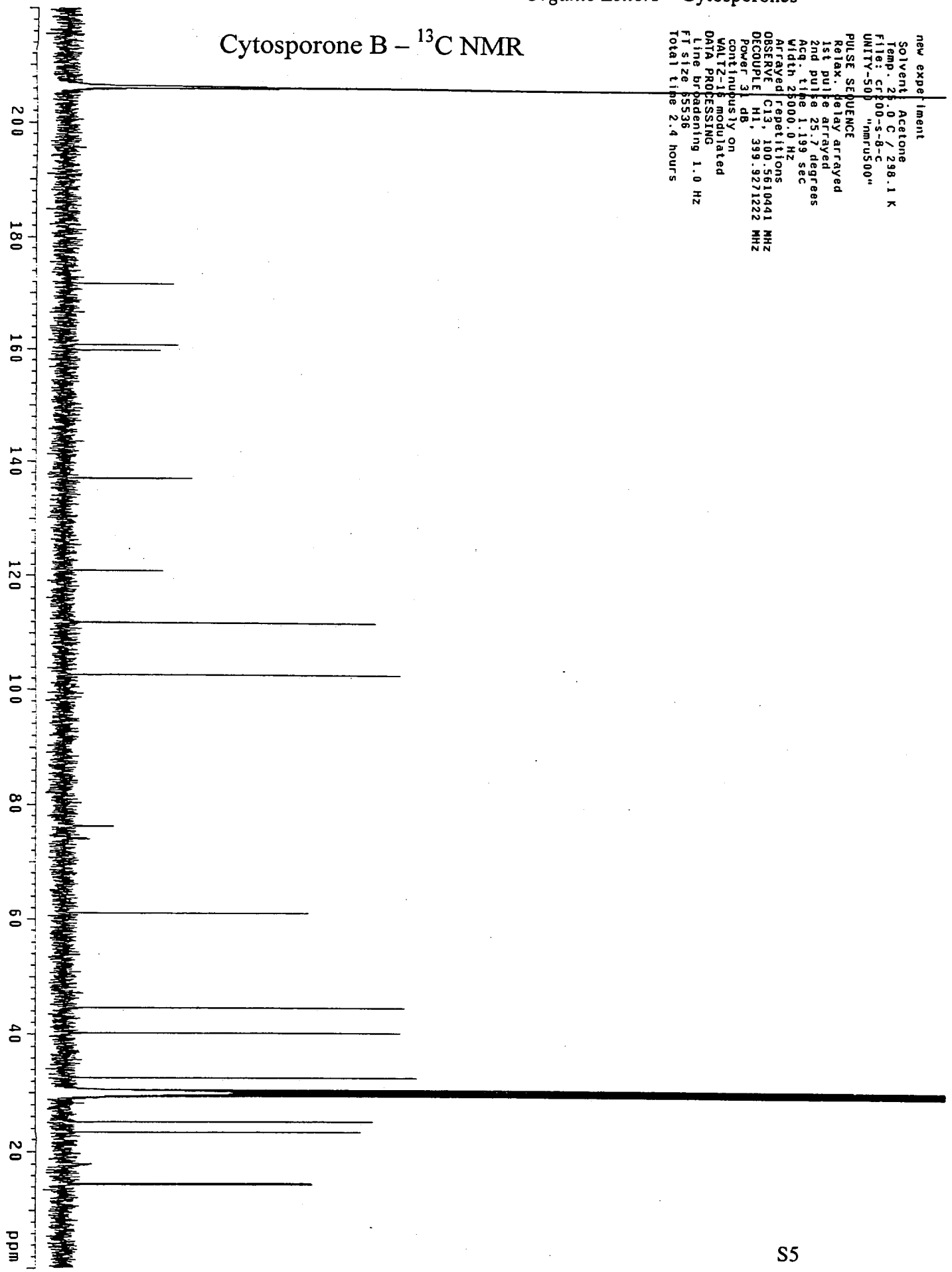
Cytosporone A – ^{1}H NMR

Cytosporone A – ^{13}C NMR

STANDARD PROTON PARAMETERS
Solvent: Acetone
Temp. 25.0 C / 298.1 K
File: cr200-s-8-H
UNITY-500 "nmru500"
PULSE SEQUENCE
Relax. delay arrayed
1st pulse arrayed
2nd pulse 51.1 degrees
Acq. time 1.888 sec
Width 3999.6 Hz
Arrayed repetitions
OBSERVE H1, 499.9270436 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 16384
Total time 3 minutes

Cytosporone B – ^{1}H NMR

Cytosporone B – ^{13}C NMR



STANDARD PROTON PARAMETERS
Solvent: Acetone
Temp. 25.0 C / 298.1 K
File: cr200-s-43B-H
UNITY-500 "nmru500"
PULSE SEQUENCE
Relax. delay arrayed
1st pulse arrayed
2nd pulse 51.1 degrees
Acq. time 1.888 sec
Width 3999.6 Hz
Arrayed repetitions
OBSERVE H1, 499.9270436 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 16384
Total time 27 minutes

Cytosporone C – ^{1}H NMR

Cytosporone C – ^{13}C NMR

Cytosporone D – ^{1}H NMR

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STANDARD PROTON PARAMETERS
  Solvent: Acetone
   Temp. 25.0 C / 298.1 K
  File: cr200s-2-H-Ace
  UNITY-500 "nmru500"
PULSE SEQUENCE
  Relax. delay arrayed
  1st pulse arrayed
  2nd pulse 51.1 degrees
  Acq. time 0.640 sec
  Width 12001.2 Hz
  Arrayed repetitions
OBSERVE    H1, 499.9270491 MHz
DATA PROCESSING
  Line broadening 0.1 Hz
  FT size 16384
  Total time 17 minutes
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Cytosporone D – ^{13}C NMR

Cytosporone E – ^{1}H NMR

Cytosporone E – ^{13}C NMR

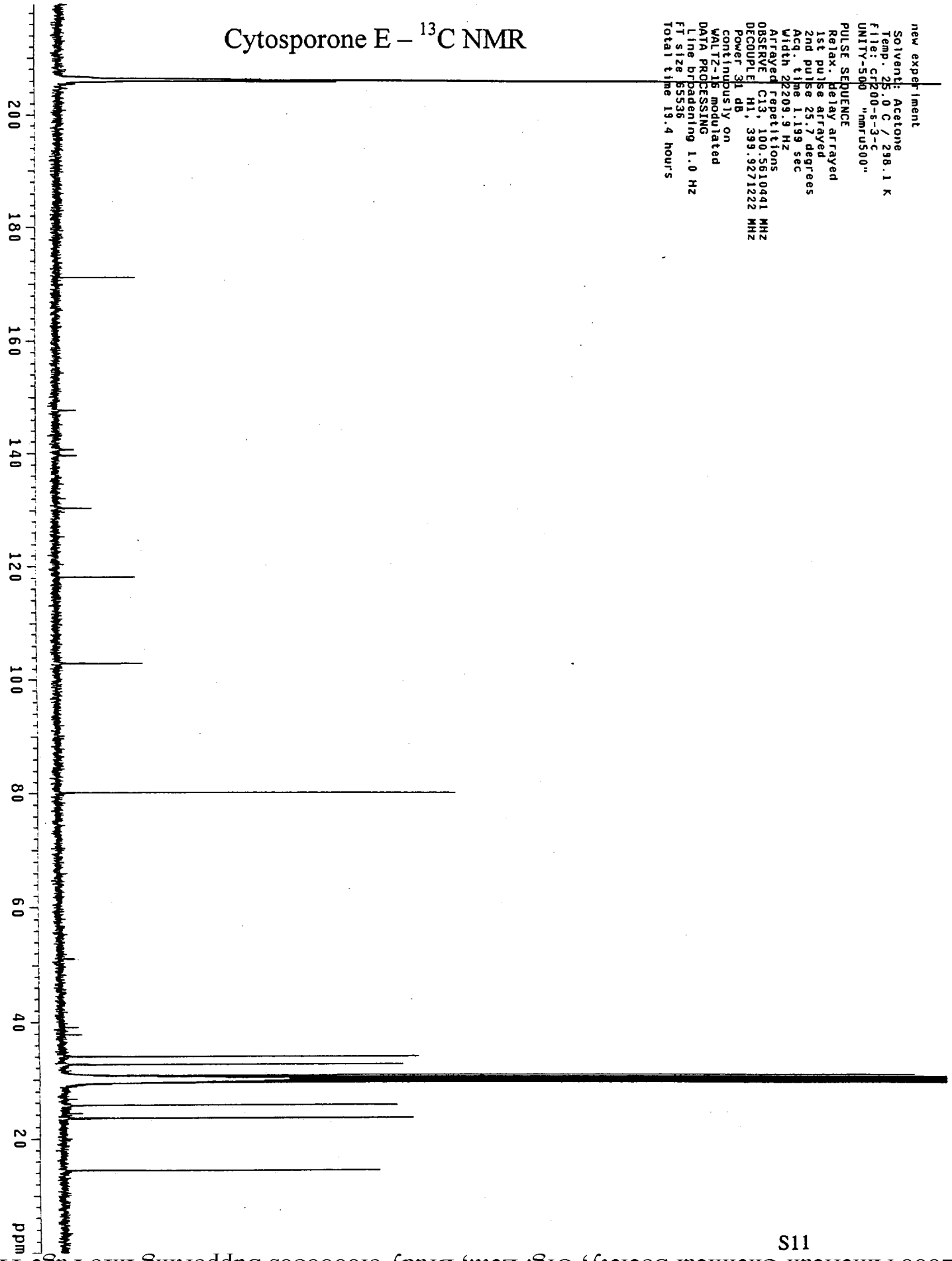

Table 1. Crystal data and structure refinement for Cytosporone C.

Identification code	Cytosporone C	
Empirical formula	C16 H24 O5	
Formula weight	296.35	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 4.8430(6) Å	α= 86.5170(4)°.
	b = 8.6725(10) Å	β= 89.810(2)°.
	c = 19.681(2) Å	γ = 77.518(2)°.
Volume	805.57(17) $Å^3$	
Z	2	
Density (calculated)	1.222 Mg/m^3	
Absorption coefficient	0.090 mm^{-1}	
F(000)	320	
Crystal size	0.4 x 0.4 x 0.05 mm^3	
Theta range for data collection	2.07 to 20.82°.	
Index ranges	-4<=h<=4, -8<=k<=7, -17<=l<=19	
Reflections collected	2714	
Independent reflections	1638 [R(int) = 0.0498]	
Completeness to theta = 20.82°	97.3 %	
Absorption correction	SADABS	
Max. and min. transmission	1 and 0.434045	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1638 / 0 / 283	
Goodness-of-fit on F^2	1.284	
Final R indices [I>2sigma(I)]	R1 = 0.0769, wR2 = 0.1969	
R indices (all data)	R1 = 0.1051, wR2 = 0.2170	
Largest diff. peak and hole	0.205 and -0.512 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	3803(10)	9593(6)	3215(3)	68(2)
O(2)	-3320(12)	3771(8)	4629(3)	60(2)
O(3)	3231(10)	2746(6)	2813(3)	65(2)
O(4)	4376(9)	7357(5)	2749(2)	45(1)
C(1)	2968(14)	8377(10)	3151(4)	52(2)
C(2)	461(17)	8066(10)	3517(6)	62(2)
C(3)	322(12)	6347(7)	3615(3)	37(2)
C(4)	-1388(13)	5854(8)	4112(3)	44(2)
C(5)	-1588(13)	4291(8)	4155(3)	40(2)
C(6)	-89(14)	3238(10)	3731(3)	47(2)
C(7)	1639(12)	3746(8)	3246(3)	41(2)
C(8)	1803(11)	5324(8)	3173(3)	37(2)
C(9)	3491(15)	5873(8)	2605(3)	44(2)
C(10)	1916(15)	6150(11)	1931(3)	46(2)
C(11)	3595(16)	6630(11)	1328(4)	53(2)
C(12)	1913(18)	6904(12)	672(4)	60(2)
C(13)	3428(18)	7485(13)	72(4)	64(2)
C(14)	1690(20)	7845(15)	-574(4)	72(3)
C(15)	3140(20)	8508(15)	-1168(5)	85(3)
C(16)	1370(30)	8960(20)	-1786(6)	109(5)
O(1S)	-4000(20)	10790(10)	4482(5)	168(4)
H(1S)	-5000	10000	5000	149(4)

Table 3. Bond lengths [Å] and angles [°] for Cytosporone C.

O(1)-C(1)	1.222(8)
O(2)-C(5)	1.372(8)
O(3)-C(7)	1.368(7)
O(4)-C(1)	1.303(8)
O(4)-C(9)	1.484(7)
C(1)-C(2)	1.476(10)
C(2)-C(3)	1.507(10)
C(3)-C(8)	1.369(8)
C(3)-C(4)	1.386(9)
C(4)-C(5)	1.377(9)
C(5)-C(6)	1.364(9)
C(6)-C(7)	1.381(9)
C(7)-C(8)	1.387(9)
C(8)-C(9)	1.497(9)
C(9)-C(10)	1.513(10)
C(10)-C(11)	1.524(9)
C(11)-C(12)	1.508(10)
C(12)-C(13)	1.506(10)
C(13)-C(14)	1.507(13)
C(14)-C(15)	1.509(12)
C(15)-C(16)	1.472(13)
O(1S)-H(1S)	1.340(8)
H(1S)-O(1S)#1	1.340(8)
C(1)-O(4)-C(9)	122.5(5)
O(1)-C(1)-O(4)	117.6(6)
O(1)-C(1)-C(2)	121.5(7)
O(4)-C(1)-C(2)	120.9(7)
C(1)-C(2)-C(3)	115.3(7)
C(8)-C(3)-C(4)	121.7(6)
C(8)-C(3)-C(2)	117.6(6)
C(4)-C(3)-C(2)	120.5(6)
C(5)-C(4)-C(3)	118.6(6)
O(2)-C(5)-C(4)	120.1(6)
O(2)-C(5)-C(6)	118.9(7)
C(4)-C(5)-C(6)	121.0(6)
C(7)-C(6)-C(5)	119.6(7)
O(3)-C(7)-C(6)	122.5(6)
O(3)-C(7)-C(8)	116.7(6)
C(6)-C(7)-C(8)	120.7(6)
C(3)-C(8)-C(7)	118.3(6)
C(3)-C(8)-C(9)	121.9(6)
C(7)-C(8)-C(9)	119.8(6)
O(4)-C(9)-C(8)	112.2(5)
O(4)-C(9)-C(10)	107.8(6)
C(8)-C(9)-C(10)	112.9(5)
C(9)-C(10)-C(11)	115.0(6)
C(12)-C(11)-C(10)	112.7(6)
C(11)-C(12)-C(13)	114.4(7)
C(14)-C(13)-C(12)	114.4(7)
C(13)-C(14)-C(15)	114.7(8)
C(16)-C(15)-C(14)	114.6(9)
O(1S)#1-H(1S)-O(1S)	179.998(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x-1,-y+2,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Cytosporone C. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	65(3)	41(3)	104(4)	-3(3)	15(3)	-29(3)
O(2)	70(4)	56(5)	62(4)	-12(3)	31(3)	-28(3)
O(3)	82(4)	40(4)	77(4)	-9(3)	40(3)	-22(3)
O(4)	44(3)	45(3)	55(3)	-5(2)	10(2)	-27(2)
C(1)	41(4)	46(5)	69(5)	4(4)	2(4)	-15(4)
C(2)	49(5)	41(5)	101(7)	-20(5)	30(5)	-19(4)
C(3)	29(4)	30(4)	53(4)	-7(3)	9(3)	-9(3)
C(4)	41(4)	45(5)	47(4)	-12(4)	13(3)	-12(4)
C(5)	41(4)	43(5)	40(4)	3(3)	11(3)	-20(4)
C(6)	55(5)	34(5)	57(5)	1(4)	9(4)	-18(4)
C(7)	44(4)	35(5)	45(4)	-7(3)	14(3)	-12(3)
C(8)	31(4)	38(5)	42(4)	3(3)	2(3)	-12(3)
C(9)	42(5)	39(5)	55(5)	-1(3)	8(4)	-19(4)
C(10)	45(5)	52(5)	48(5)	-2(4)	8(4)	-25(5)
C(11)	50(5)	62(6)	49(5)	-3(4)	9(4)	-21(5)
C(12)	61(5)	74(7)	51(5)	-1(4)	7(4)	-31(5)
C(13)	59(5)	82(7)	54(5)	2(4)	14(4)	-24(5)
C(14)	64(7)	98(8)	56(6)	-3(5)	9(5)	-24(6)
C(15)	68(6)	126(9)	57(6)	11(6)	9(5)	-19(7)
C(16)	97(9)	151(14)	66(7)	23(7)	22(7)	-7(8)
O(1S)	231(9)	117(7)	174(8)	-1(5)	77(8)	-77(6)

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

	x	y	z	U(eq)
H(2O)	-3410(140)	4360(80)	4790(30)	40(20)
H(3O)	3310(110)	1720(80)	2960(30)	34(17)
H(2B)	-1220(170)	8730(90)	3220(40)	70(30)
H(2A)	80(160)	8460(90)	3910(40)	70(30)
H(4A)	-2420(120)	6620(70)	4420(30)	45(17)
H(6A)	-190(110)	2260(80)	3780(30)	26(18)
H(9A)	5490(150)	5230(80)	2610(30)	50(20)
H(10B)	60(150)	7040(80)	1960(30)	50(20)
H(10A)	1410(110)	5260(80)	1820(30)	42(18)
H(11B)	5410(170)	5760(100)	1290(40)	80(30)
H(11A)	3960(160)	7650(110)	1450(40)	90(30)
H(12B)	160(180)	7770(100)	700(40)	90(30)
H(12A)	1250(140)	5970(90)	550(30)	60(20)
H(13B)	5230(160)	6720(90)	-40(30)	70(20)
H(13A)	4210(190)	8200(110)	120(40)	110(40)
H(14B)	-30(170)	8500(90)	-580(40)	100(30)
H(14A)	1290(170)	6920(110)	-750(40)	100(30)
H(15B)	5000(200)	7710(110)	-1260(40)	110(30)
H(15A)	4500(200)	9170(120)	-1130(50)	140(40)
H(16C)	900(400)	8100(200)	-1900(80)	170(100)
H(16B)	2490(170)	9320(100)	-2120(50)	100(30)
H(16A)	-600(200)	9510(120)	-1660(50)	110(40)
H(2S)	-1840(100)	10520(60)	5120(30)	42(15)