Supplementary Material for

The Guanacastepenes: A Highly Diverse Family of Secondary Metabolites Produced by an Endophytic Fungus

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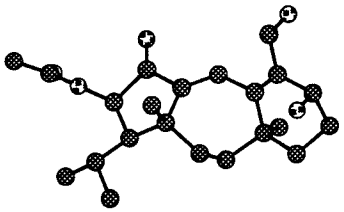
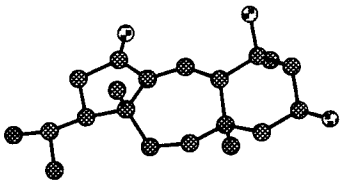
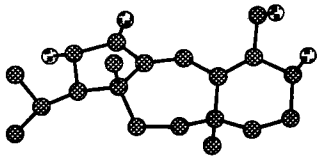


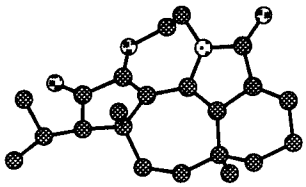
Guanacastepene A
+93.6°



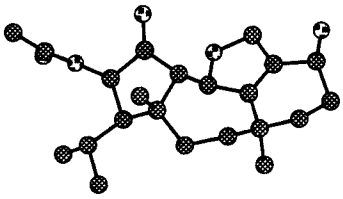
Guanacastepene B
-76.5°



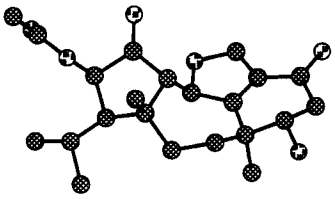
Guanacastepene C
-77.3°



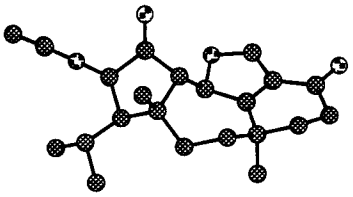
Guanacastepene D
-73.6°



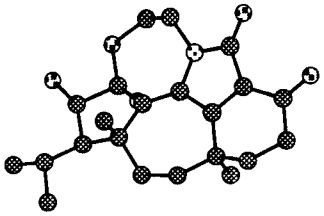
GuanacastepeneE
-88.5°



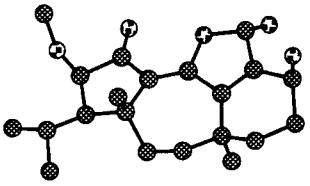
Guanacastepene F
-92.0°



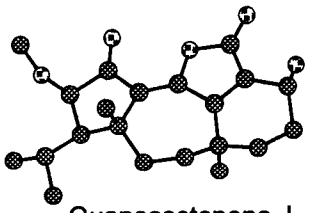
Guanacastepene G
-93.0°



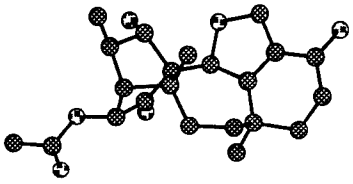
Guanacastepene H
-71.6°



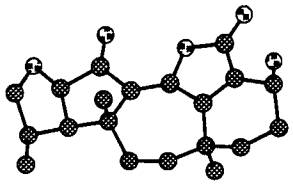
Guanacastepene I
-87.5°



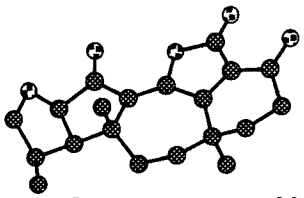
Guanacastepene J
-84.2°



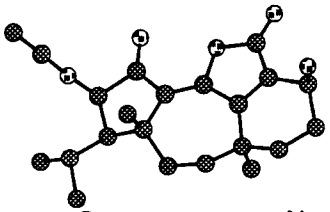
Guanacastepene K
-68.4°



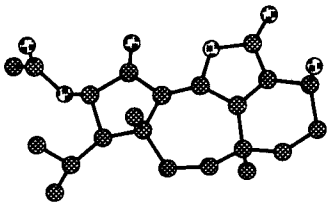
GuanacastepeneL
-76.2°



Guanacastepene M
-78.0°



Guanacastepene N
-79.7°



Guanacastepene O
-80.0°

Dihedral angles for the C-8-9-10-11 bond in the X-ray crystal structures of the guanacastepenes. The C-8-9-10-11 bond crystallizes in the opposite gauche butane-like conformation in guanacastepene A than it does the other guanacastepenes.

rDNA was amplified from crude CR115 DNA with primers ITS 1 and ITS 4 using the polymerase chain reaction and then the gel purified PCR product was directly sequenced with ITS1, ITS2, ITS3 and ITS4. The following sequence, derived from sequencing four independent PCR products with all four primers, was used in the BLAST search against deposited sequences.

CR115 internal transcribed spacers (ITS1 and ITS2) and 5.8S rDNA gene sequence.

5'-TTCCTCCCGCTTATTGATATGCTTAAGTTCAGCGGGTAGTCCTACCTGAT
TTGAGGTCAAATTGGTCAAGTAGATTGTCCTCGCGGACGGTTAGAAGCGA
GCATGAGTCCAAATCCACGGCGTAGATAATTATCACACCAATAGACGGAA
GCTCAGTATGAGCTCGCTAATGCATTTCAGGGGAGCAGACCAGCACTGAG
GCAGCCTGCAAAGACCCCCACATCCAAGCCTTCACCGGTTTCGTTACAAA
ACTGGTGAGGTTGAGAATTTAATGACACTCAAACAGGCATGCTCCTCGGA
ATACCAAGGAGCGCAAGGTGCGTTCAAAGATTCGATGATTCACTGAATTC
TGCAATTCACATTACTTATCGCATTTCGCTGCGTTCTTCATCGATGCGAG
AGCCAAGAGATCCGTTGCTGAAAGTTGTATAGTGGTTTATAGGCATGGAA
GCCCATTGACTACATTCTACATCATTCAAATGGGGTGTGTAAAAGACATA
GAACCTGGAAATTCAAAGAGAGTTGGCCTTATCGACGCAGCAATCCTTGT
ATCCGCTCTAGAGCGAGGGGTATCCAGGCCTACACATAGTTCACAGGTGG
AAAGATGATATGAATGACGGGCGTGCACAAATGCTCCTAGGAGCCAGCTA
CAACCAACGCCATAGATATTCGTTAATGATCCTTCCGCAGGTTCACCTTA
CGGAAG-3'

Table 1. Crystal data and structure refinement for guanacastepene B.

Identification code	sean27	
Empirical formula	C23 H42 O6	
Formula weight	414.57	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 8.1474(8) Å	α= 90°.
	b = 7.7262(8) Å	β= 101.039(2)°.
	c = 19.0037(18) Å	γ = 90°.
Volume	1174.1(2) $Å^3$	
Z	2	
Density (calculated)	1.173 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	456	
Crystal size	0.40 x 0.10 x 0.05 mm^3	
Theta range for data collection	1.09 to 28.28°.	
Index ranges	-10<=h<=10, -10<=k<=10, -25<=l<=25	
Reflections collected	11087	
Independent reflections	5532 [R(int) = 0.0493]	
Completeness to theta = 28.28°	99.1 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9959 and 0.575769	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5532 / 1 / 419	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0479, wR2 = 0.0995	
R indices (all data)	R1 = 0.0643, wR2 = 0.1069	
Absolute structure parameter	0.4(9)	
Largest diff. peak and hole	0.285 and -0.240 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	2453(2)	11783(2)	1346(1)	20(1)
O(2)	5231(2)	6757(2)	601(1)	25(1)
O(3)	2691(2)	13490(2)	3791(1)	38(1)
C(1)	2940(2)	10490(2)	3475(1)	16(1)
C(2)	3282(2)	10814(2)	2829(1)	17(1)
C(3)	3504(2)	9582(2)	2239(1)	14(1)
C(4)	3849(2)	10618(2)	1578(1)	17(1)
C(5)	3945(3)	9352(3)	967(1)	19(1)
C(6)	5229(3)	7945(3)	1186(1)	18(1)
C(7)	4823(3)	6918(3)	1813(1)	19(1)
C(8)	4727(2)	8034(2)	2475(1)	16(1)
C(9)	3993(3)	6828(3)	2986(1)	17(1)
C(10)	4001(3)	7449(3)	3751(1)	17(1)
C(11)	2679(2)	8795(2)	3844(1)	15(1)
C(12)	2857(2)	9343(3)	4660(1)	16(1)
C(13)	2305(3)	11242(3)	4634(1)	21(1)
C(14)	2663(3)	11976(3)	3940(1)	21(1)
C(15)	5374(3)	11796(3)	1729(1)	22(1)
C(16)	6498(2)	8593(3)	2840(1)	20(1)
C(17)	890(3)	8157(3)	3546(1)	21(1)
C(18)	1955(3)	8237(3)	5142(1)	19(1)
C(19)	2209(4)	9038(3)	5898(1)	33(1)
C(20)	2495(3)	6348(3)	5214(1)	24(1)
O(1W)	3064(2)	13940(2)	220(1)	25(1)
O(2W)	9512(2)	-132(3)	968(1)	40(1)
O(1S)	9803(3)	6759(3)	1729(1)	64(1)
C(1S)	9492(3)	5250(3)	1605(1)	32(1)
C(2S)	8962(4)	4592(5)	857(2)	45(1)
C(3S)	9561(3)	3986(4)	2199(1)	40(1)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene B.

O(1)-C(4)	1.451(2)
O(2)-C(6)	1.442(2)
O(3)-C(14)	1.204(3)
C(1)-C(2)	1.333(3)
C(1)-C(14)	1.492(3)
C(1)-C(11)	1.520(3)
C(2)-C(3)	1.507(3)
C(3)-C(4)	1.560(2)
C(3)-C(8)	1.567(3)
C(4)-C(15)	1.522(3)
C(4)-C(5)	1.532(3)
C(5)-C(6)	1.511(3)
C(6)-C(7)	1.520(3)
C(7)-C(8)	1.539(2)
C(8)-C(16)	1.538(3)
C(8)-C(9)	1.546(3)
C(9)-C(10)	1.530(2)
C(10)-C(11)	1.531(3)
C(11)-C(17)	1.540(3)
C(11)-C(12)	1.589(2)
C(12)-C(13)	1.533(3)
C(12)-C(18)	1.538(3)
C(13)-C(14)	1.515(3)
C(18)-C(20)	1.523(3)
C(18)-C(19)	1.540(3)
O(1S)-C(1S)	1.207(3)
C(1S)-C(3S)	1.486(3)
C(1S)-C(2S)	1.494(3)
C(2)-C(1)-C(14)	118.90(18)
C(2)-C(1)-C(11)	131.20(18)
C(14)-C(1)-C(11)	109.83(15)
C(1)-C(2)-C(3)	129.93(18)
C(2)-C(3)-C(4)	109.91(15)
C(2)-C(3)-C(8)	115.46(14)
C(4)-C(3)-C(8)	114.77(15)
O(1)-C(4)-C(15)	104.52(16)
O(1)-C(4)-C(5)	108.42(14)
C(15)-C(4)-C(5)	111.51(17)
O(1)-C(4)-C(3)	108.15(15)
C(15)-C(4)-C(3)	114.91(15)
C(5)-C(4)-C(3)	109.03(15)
C(6)-C(5)-C(4)	112.57(15)
O(2)-C(6)-C(5)	110.39(15)
O(2)-C(6)-C(7)	107.76(15)
C(5)-C(6)-C(7)	110.38(16)
C(6)-C(7)-C(8)	113.65(16)
C(16)-C(8)-C(7)	109.62(16)
C(16)-C(8)-C(9)	109.20(15)
C(7)-C(8)-C(9)	105.15(15)
C(16)-C(8)-C(3)	113.88(16)
C(7)-C(8)-C(3)	108.86(14)
C(9)-C(8)-C(3)	109.77(15)
C(10)-C(9)-C(8)	118.39(16)
C(11)-C(10)-C(9)	116.58(15)
C(1)-C(11)-C(10)	111.59(15)

C(1)-C(11)-C(17)	108.21(16)
C(10)-C(11)-C(17)	112.18(16)
C(1)-C(11)-C(12)	103.08(14)
C(10)-C(11)-C(12)	111.04(15)
C(17)-C(11)-C(12)	110.35(15)
C(13)-C(12)-C(18)	112.36(15)
C(13)-C(12)-C(11)	104.62(15)
C(18)-C(12)-C(11)	117.96(16)
C(14)-C(13)-C(12)	106.40(15)
O(3)-C(14)-C(1)	126.63(18)
O(3)-C(14)-C(13)	125.64(18)
C(1)-C(14)-C(13)	107.72(17)
C(20)-C(18)-C(12)	115.03(16)
C(20)-C(18)-C(19)	108.44(18)
C(12)-C(18)-C(19)	109.72(17)
O(1S)-C(1S)-C(3S)	120.7(2)
O(1S)-C(1S)-C(2S)	121.8(2)
C(3S)-C(1S)-C(2S)	117.5(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for guanacastepene B. 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)	20(1)	21(1)	18(1)	4(1)	4(1)	2(1)
O(2)	34(1)	25(1)	18(1)	-4(1)	14(1)	-4(1)
O(3)	69(1)	19(1)	31(1)	-4(1)	23(1)	-1(1)
C(1)	16(1)	16(1)	16(1)	-2(1)	1(1)	0(1)
C(2)	16(1)	15(1)	18(1)	0(1)	2(1)	1(1)
C(3)	15(1)	15(1)	13(1)	-1(1)	4(1)	-2(1)
C(4)	19(1)	16(1)	15(1)	2(1)	4(1)	2(1)
C(5)	21(1)	25(1)	13(1)	2(1)	7(1)	-1(1)
C(6)	19(1)	20(1)	15(1)	-3(1)	7(1)	-2(1)
C(7)	24(1)	18(1)	15(1)	1(1)	7(1)	2(1)
C(8)	18(1)	17(1)	14(1)	1(1)	4(1)	2(1)
C(9)	22(1)	14(1)	15(1)	0(1)	7(1)	3(1)
C(10)	19(1)	18(1)	14(1)	2(1)	4(1)	0(1)
C(11)	17(1)	18(1)	11(1)	-1(1)	3(1)	-1(1)
C(12)	15(1)	22(1)	12(1)	-4(1)	3(1)	-1(1)
C(13)	23(1)	22(1)	19(1)	-6(1)	7(1)	-3(1)
C(14)	25(1)	22(1)	19(1)	-5(1)	7(1)	-1(1)
C(15)	24(1)	21(1)	24(1)	2(1)	9(1)	-4(1)
C(16)	16(1)	26(1)	18(1)	1(1)	1(1)	1(1)
C(17)	18(1)	26(1)	17(1)	-3(1)	1(1)	-4(1)
C(18)	19(1)	25(1)	16(1)	-2(1)	7(1)	-1(1)
C(19)	49(2)	35(2)	19(1)	-4(1)	16(1)	-5(1)
C(20)	28(1)	27(1)	19(1)	3(1)	9(1)	-1(1)
O(1W)	31(1)	27(1)	18(1)	2(1)	7(1)	-4(1)
O(2W)	35(1)	41(1)	39(1)	6(1)	-6(1)	-8(1)
O(1S)	94(2)	48(1)	38(1)	10(1)	-17(1)	-31(1)
C(1S)	22(1)	43(2)	29(1)	1(1)	1(1)	-6(1)
C(2S)	45(2)	56(2)	32(1)	-6(1)	0(1)	17(2)
C(3S)	40(2)	43(2)	36(1)	2(1)	6(1)	-2(1)

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

	x	y	z	U(eq)
H(1O)	1610(40)	11240(40)	1175(16)	58(10)
H(2O)	5670(40)	7230(40)	295(16)	57(10)
H(2)	3360(20)	12040(30)	2728(10)	8(5)
H(3)	2400(20)	9070(20)	2063(9)	3(4)
H(5B)	4250(30)	9970(30)	587(10)	12(5)
H(5A)	2890(30)	8770(30)	797(12)	26(6)
H(6)	6330(20)	8490(30)	1317(10)	8(5)
H(7B)	3700(30)	6320(30)	1630(13)	36(7)
H(7A)	5610(30)	6010(30)	1954(11)	15(5)
H(9B)	2820(30)	6590(30)	2743(10)	13(5)
H(9A)	4680(30)	5800(30)	3009(10)	13(5)
H(10B)	5100(30)	7850(30)	3969(11)	14(5)
H(10A)	3770(30)	6490(30)	3998(11)	22(6)
H(12)	4070(30)	9260(30)	4871(10)	19(5)
H(13B)	2900(30)	11950(40)	5075(13)	38(7)
H(13A)	1120(30)	11310(30)	4577(11)	24(6)
H(15C)	5430(30)	12580(40)	2181(14)	44(7)
H(15B)	6460(30)	11080(30)	1797(12)	35(7)
H(15A)	5400(30)	12510(30)	1326(13)	33(6)
H(16C)	6470(30)	9560(30)	3167(11)	24(6)
H(16B)	7210(30)	9010(30)	2476(11)	24(6)
H(16A)	7110(20)	7660(30)	3108(10)	12(5)
H(17C)	680(30)	7010(30)	3718(11)	23(6)
H(17B)	670(30)	8010(30)	3014(12)	23(6)
H(17A)	60(30)	8940(30)	3659(12)	27(6)
H(18)	750(30)	8240(30)	4936(12)	24(6)
H(19C)	3400(40)	9010(40)	6122(16)	60(9)
H(19B)	1800(30)	10150(30)	5865(12)	27(6)
H(19A)	1560(40)	8310(40)	6213(15)	53(9)
H(20C)	2190(30)	5630(30)	4761(13)	32(7)
H(20B)	3750(40)	6280(30)	5376(14)	46(8)
H(20A)	1880(30)	5670(30)	5569(12)	27(6)
H(1WB)	2840(40)	13430(40)	485(16)	48(10)
H(1WA)	3630(30)	14790(40)	355(12)	25(7)
H(2WB)	9550(30)	-1070(40)	1165(13)	26(7)
H(2WA)	8860(50)	-310(50)	600(20)	79(13)
H(2SC)	9060(50)	5450(50)	510(20)	82(12)
H(2SB)	9570(50)	3680(50)	790(20)	85(13)
H(2SA)	7840(50)	4430(50)	764(19)	82(12)
H(3SC)	10591(19)	3848(5)	2415(4)	60
H(3SB)	9158(8)	3002(19)	2028(3)	60
H(3SA)	8976(11)	4370(8)	2502(6)	60

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

Identification code	hp1-b	
Empirical formula	C20 H32.50 O4.50	
Formula weight	344.96	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 13.1534(8) Å	α= 90°.
	b = 25.3159(16) Å	β= 119.297(3)°.
	c = 13.1690(8) Å	γ = 90°.
Volume	3824.3(4) $Å^3$	
Z	8	
Density (calculated)	1.198 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	1508	
Crystal size	0.30 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.39 to 20.82°.	
Index ranges	-13<=h<=13, -25<=k<=25, -13<=l<=12	
Reflections collected	20978	
Independent reflections	7994 [R(int) = 0.0686]	
Completeness to theta = 20.82°	99.8 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9918 and 0.781550	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7994 / 1 / 971	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0595, wR2 = 0.1102	
R indices (all data)	R1 = 0.0881, wR2 = 0.1196	
Absolute structure parameter	0.9(13)	
Largest diff. peak and hole	0.187 and -0.184 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	9338(3)	8024(2)	6469(4)	27(1)
O(2)	11796(4)	8964(2)	7007(4)	32(1)
O(3)	12555(4)	8938(2)	3574(4)	37(1)
O(4)	12987(4)	8452(2)	1915(4)	47(1)
C(1)	11428(4)	8157(2)	3450(5)	18(2)
C(2)	11425(5)	8244(2)	4453(5)	24(2)
C(3)	11002(5)	7933(2)	5105(5)	20(2)
C(4)	10774(5)	8193(2)	5874(5)	21(2)
C(5)	10526(5)	7920(2)	6745(5)	23(2)
C(6)	10753(5)	7332(2)	6841(5)	26(2)
C(7)	10345(5)	7098(2)	5625(5)	26(2)
C(8)	11017(5)	7335(2)	5051(5)	19(2)
C(9)	10382(6)	7122(3)	3799(6)	29(2)
C(10)	10978(5)	7186(2)	3037(5)	26(2)
C(11)	10910(5)	7736(2)	2529(5)	22(2)
C(12)	11658(5)	7763(2)	1909(5)	27(2)
C(13)	11954(5)	8347(2)	1947(5)	23(2)
C(14)	12037(5)	8540(2)	3076(6)	27(2)
C(15)	10783(5)	8789(2)	5962(5)	26(2)
C(16)	12278(5)	7144(2)	5684(5)	25(2)
C(17)	9633(5)	7879(3)	1689(5)	34(2)
C(18)	11235(6)	7473(3)	758(6)	42(2)
C(19)	10545(6)	7813(3)	-309(6)	55(2)
C(20)	12271(7)	7229(3)	675(7)	57(2)
O(1A)	6202(4)	9855(2)	3184(4)	35(1)
O(2A)	5846(4)	8981(2)	938(4)	38(1)
O(3A)	9236(4)	9106(2)	-38(4)	42(1)
O(4A)	10704(4)	9642(2)	-646(4)	54(2)
C(1A)	9328(5)	9890(2)	1067(5)	22(2)
C(2A)	8358(5)	9766(2)	1110(5)	22(2)
C(3A)	7686(5)	10053(2)	1581(5)	25(2)
C(4A)	6973(5)	9773(2)	1822(5)	26(2)
C(5A)	6063(5)	10021(2)	2065(5)	32(2)
C(6A)	5972(5)	10607(2)	1939(6)	35(2)
C(7A)	7157(5)	10854(2)	2305(6)	30(2)
C(8A)	7702(5)	10657(2)	1577(5)	24(2)
C(9A)	8918(6)	10904(3)	2142(7)	34(2)
C(10A)	9636(5)	10870(2)	1503(6)	36(2)
C(11A)	10190(5)	10336(2)	1534(5)	26(2)
C(12A)	10722(5)	10334(3)	708(6)	36(2)
C(13A)	10760(5)	9749(3)	445(6)	36(2)
C(14A)	9704(5)	9518(3)	448(6)	34(2)
C(15A)	6943(6)	9177(2)	1835(6)	33(2)
C(16A)	6967(5)	10845(2)	292(6)	33(2)
C(17A)	11116(6)	10206(3)	2815(5)	45(2)
C(18A)	11829(6)	10662(3)	1066(7)	61(2)
C(19A)	12973(6)	10342(4)	1760(8)	90(3)
C(20A)	11776(8)	10928(4)	5(8)	100(4)
O(1B)	8265(3)	9592(2)	5095(4)	31(1)
O(2B)	9274(3)	8857(2)	7741(3)	33(1)
O(3B)	5811(3)	9384(2)	9004(4)	35(1)
O(4B)	4088(4)	10087(2)	9005(4)	37(1)
C(1B)	5637(5)	9936(2)	7422(5)	19(2)

C(2B)	6700(5)	9806(2)	7559(5)	24(2)
C(3B)	7318(5)	9976(2)	6939(5)	21(2)
C(4B)	8035(5)	9627(2)	6823(5)	23(2)
C(5B)	8785(5)	9785(3)	6291(5)	28(2)
C(6B)	8945(5)	10365(2)	6274(6)	34(2)
C(7B)	7788(5)	10641(3)	5798(6)	38(2)
C(8B)	7148(5)	10549(2)	6502(5)	25(2)
C(9B)	5840(6)	10673(3)	5636(6)	34(2)
C(10B)	5016(5)	10755(2)	6140(6)	31(2)
C(11B)	4641(5)	10269(2)	6530(5)	23(2)
C(12B)	4020(5)	10429(2)	7219(5)	27(2)
C(13B)	4120(5)	9949(2)	7962(5)	25(2)
C(14B)	5273(5)	9711(2)	8235(5)	24(2)
C(15B)	8124(5)	9055(2)	7177(5)	28(2)
C(16B)	7631(6)	10924(3)	7528(6)	42(2)
C(17B)	3876(5)	9911(2)	5482(5)	33(2)
C(18B)	2788(5)	10677(3)	6507(6)	34(2)
C(19B)	1797(5)	10291(3)	6134(6)	53(2)
C(20B)	2611(7)	11138(3)	7146(6)	63(2)
O(1C)	7611(4)	8496(2)	4438(4)	32(1)
O(2C)	4751(4)	9121(2)	3260(4)	40(1)
O(3C)	3646(3)	8643(2)	6751(3)	28(1)
O(4C)	3610(4)	7962(2)	8466(4)	35(1)
C(1C)	5169(5)	8070(2)	6886(5)	19(2)
C(2C)	5049(5)	8217(2)	5856(5)	19(2)
C(3C)	5684(5)	8053(2)	5220(5)	25(2)
C(4C)	5846(5)	8408(2)	4548(5)	26(2)
C(5C)	6437(5)	8271(2)	3855(6)	28(2)
C(6C)	6421(6)	7694(2)	3613(6)	35(2)
C(7C)	6790(6)	7380(2)	4711(6)	34(2)
C(8C)	6046(5)	7467(2)	5311(5)	24(2)
C(9C)	6797(7)	7257(3)	6555(7)	39(2)
C(10C)	6210(6)	7182(2)	7306(6)	35(2)
C(11C)	5988(5)	7685(2)	7814(5)	23(2)
C(12C)	5296(5)	7554(2)	8456(5)	24(2)
C(13C)	4652(5)	8055(2)	8420(5)	20(2)
C(14C)	4393(5)	8302(2)	7261(5)	20(2)
C(15C)	5477(5)	8979(2)	4457(5)	26(2)
C(16C)	4890(6)	7153(2)	4628(6)	43(2)
C(17C)	7144(4)	7987(3)	8600(5)	36(2)
C(18C)	5974(5)	7280(2)	9651(6)	32(2)
C(19C)	6481(6)	7649(3)	10700(6)	49(2)
C(20C)	5207(7)	6876(3)	9812(7)	64(2)
O(2W)	2565(5)	9365(2)	9165(6)	45(2)
O(1W)	13850(4)	8500(2)	407(4)	49(2)

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

O(1)-C(5)	1.444(6)
O(2)-C(15)	1.439(7)
O(3)-C(14)	1.213(7)
O(4)-C(13)	1.405(7)
C(1)-C(2)	1.340(7)
C(1)-C(14)	1.487(8)
C(1)-C(11)	1.505(8)
C(2)-C(3)	1.459(8)
C(3)-C(4)	1.359(7)
C(3)-C(8)	1.517(8)
C(4)-C(5)	1.506(8)
C(4)-C(15)	1.511(8)
C(5)-C(6)	1.512(7)
C(6)-C(7)	1.536(8)
C(7)-C(8)	1.538(8)
C(8)-C(16)	1.525(7)
C(8)-C(9)	1.536(9)
C(9)-C(10)	1.554(8)
C(10)-C(11)	1.528(7)
C(11)-C(17)	1.536(8)
C(11)-C(12)	1.558(8)
C(12)-C(13)	1.523(8)
C(12)-C(18)	1.524(9)
C(13)-C(14)	1.518(8)
C(18)-C(19)	1.515(9)
C(18)-C(20)	1.548(9)
O(1A)-C(5A)	1.455(7)
O(2A)-C(15A)	1.434(7)
O(3A)-C(14A)	1.221(7)
O(4A)-C(13A)	1.428(7)
C(1A)-C(2A)	1.342(7)
C(1A)-C(14A)	1.480(8)
C(1A)-C(11A)	1.503(8)
C(2A)-C(3A)	1.493(8)
C(3A)-C(4A)	1.332(8)
C(3A)-C(8A)	1.530(8)
C(4A)-C(15A)	1.509(8)
C(4A)-C(5A)	1.517(8)
C(5A)-C(6A)	1.491(8)
C(6A)-C(7A)	1.523(8)
C(7A)-C(8A)	1.535(8)
C(8A)-C(9A)	1.530(8)
C(8A)-C(16A)	1.557(8)
C(9A)-C(10A)	1.544(8)
C(10A)-C(11A)	1.526(8)
C(11A)-C(12A)	1.554(8)
C(11A)-C(17A)	1.558(8)
C(12A)-C(13A)	1.526(9)
C(12A)-C(18A)	1.537(9)
C(13A)-C(14A)	1.511(9)
C(18A)-C(20A)	1.522(10)
C(18A)-C(19A)	1.552(10)
O(1B)-C(5B)	1.461(7)
O(2B)-C(15B)	1.411(6)
O(3B)-C(14B)	1.228(7)
O(4B)-C(13B)	1.437(7)

C(1B)-C(2B)	1.361(7)
C(1B)-C(14B)	1.484(8)
C(1B)-C(11B)	1.516(8)
C(2B)-C(3B)	1.470(8)
C(3B)-C(4B)	1.354(7)
C(3B)-C(8B)	1.535(8)
C(4B)-C(15B)	1.508(8)
C(4B)-C(5B)	1.517(8)
C(5B)-C(6B)	1.484(8)
C(6B)-C(7B)	1.505(8)
C(7B)-C(8B)	1.544(8)
C(8B)-C(16B)	1.514(8)
C(8B)-C(9B)	1.562(9)
C(9B)-C(10B)	1.536(8)
C(10B)-C(11B)	1.507(7)
C(11B)-C(17B)	1.542(8)
C(11B)-C(12B)	1.543(8)
C(12B)-C(13B)	1.523(8)
C(12B)-C(18B)	1.553(8)
C(13B)-C(14B)	1.503(8)
C(18B)-C(19B)	1.506(8)
C(18B)-C(20B)	1.521(8)
O(1C)-C(5C)	1.463(7)
O(2C)-C(15C)	1.432(7)
O(3C)-C(14C)	1.232(6)
O(4C)-C(13C)	1.422(6)
C(1C)-C(2C)	1.340(7)
C(1C)-C(14C)	1.457(8)
C(1C)-C(11C)	1.522(8)
C(2C)-C(3C)	1.501(8)
C(3C)-C(4C)	1.348(8)
C(3C)-C(8C)	1.544(8)
C(4C)-C(5C)	1.500(8)
C(4C)-C(15C)	1.511(8)
C(5C)-C(6C)	1.492(8)
C(6C)-C(7C)	1.509(8)
C(7C)-C(8C)	1.546(8)
C(8C)-C(9C)	1.536(9)
C(8C)-C(16C)	1.554(8)
C(9C)-C(10C)	1.535(8)
C(10C)-C(11C)	1.531(8)
C(11C)-C(12C)	1.550(7)
C(11C)-C(17C)	1.559(8)
C(12C)-C(13C)	1.513(8)
C(12C)-C(18C)	1.543(8)
C(13C)-C(14C)	1.525(8)
C(18C)-C(20C)	1.521(8)
C(18C)-C(19C)	1.524(9)

C(2)-C(1)-C(14)	118.8(5)
C(2)-C(1)-C(11)	133.7(5)
C(14)-C(1)-C(11)	107.4(5)
C(1)-C(2)-C(3)	132.6(6)
C(4)-C(3)-C(2)	117.7(5)
C(4)-C(3)-C(8)	122.0(5)
C(2)-C(3)-C(8)	119.5(5)
C(3)-C(4)-C(5)	123.7(5)
C(3)-C(4)-C(15)	122.9(5)

C(5)-C(4)-C(15)	113.4(5)
O(1)-C(5)-C(4)	109.6(4)
O(1)-C(5)-C(6)	110.3(5)
C(4)-C(5)-C(6)	114.1(5)
C(5)-C(6)-C(7)	109.8(5)
C(6)-C(7)-C(8)	111.7(5)
C(3)-C(8)-C(16)	109.0(5)
C(3)-C(8)-C(9)	112.8(5)
C(16)-C(8)-C(9)	110.5(5)
C(3)-C(8)-C(7)	110.1(5)
C(16)-C(8)-C(7)	109.9(5)
C(9)-C(8)-C(7)	104.5(4)
C(8)-C(9)-C(10)	118.4(5)
C(11)-C(10)-C(9)	115.9(5)
C(1)-C(11)-C(10)	112.7(5)
C(1)-C(11)-C(17)	108.5(5)
C(10)-C(11)-C(17)	109.9(5)
C(1)-C(11)-C(12)	103.8(4)
C(10)-C(11)-C(12)	110.7(5)
C(17)-C(11)-C(12)	111.1(5)
C(13)-C(12)-C(18)	117.7(5)
C(13)-C(12)-C(11)	104.0(5)
C(18)-C(12)-C(11)	118.9(5)
O(4)-C(13)-C(14)	111.2(5)
O(4)-C(13)-C(12)	114.7(5)
C(14)-C(13)-C(12)	103.9(5)
O(3)-C(14)-C(1)	127.8(6)
O(3)-C(14)-C(13)	123.3(5)
C(1)-C(14)-C(13)	108.8(5)
O(2)-C(15)-C(4)	110.5(5)
C(19)-C(18)-C(12)	114.2(6)
C(19)-C(18)-C(20)	108.0(6)
C(12)-C(18)-C(20)	110.9(6)
C(2A)-C(1A)-C(14A)	117.1(5)
C(2A)-C(1A)-C(11A)	134.5(5)
C(14A)-C(1A)-C(11A)	108.4(5)
C(1A)-C(2A)-C(3A)	132.2(5)
C(4A)-C(3A)-C(2A)	118.0(5)
C(4A)-C(3A)-C(8A)	123.0(5)
C(2A)-C(3A)-C(8A)	118.2(5)
C(3A)-C(4A)-C(15A)	124.0(5)
C(3A)-C(4A)-C(5A)	123.4(5)
C(15A)-C(4A)-C(5A)	112.5(5)
O(1A)-C(5A)-C(6A)	111.4(5)
O(1A)-C(5A)-C(4A)	111.8(5)
C(6A)-C(5A)-C(4A)	114.6(5)
C(5A)-C(6A)-C(7A)	111.1(5)
C(6A)-C(7A)-C(8A)	112.7(5)
C(3A)-C(8A)-C(9A)	114.9(5)
C(3A)-C(8A)-C(7A)	108.2(5)
C(9A)-C(8A)-C(7A)	105.1(5)
C(3A)-C(8A)-C(16A)	107.9(5)
C(9A)-C(8A)-C(16A)	110.4(5)
C(7A)-C(8A)-C(16A)	110.4(5)
C(8A)-C(9A)-C(10A)	119.0(6)
C(11A)-C(10A)-C(9A)	116.5(5)
C(1A)-C(11A)-C(10A)	113.6(5)
C(1A)-C(11A)-C(12A)	102.6(5)

C(10A)-C(11A)-C(12A)	110.9(5)
C(1A)-C(11A)-C(17A)	108.5(5)
C(10A)-C(11A)-C(17A)	109.1(5)
C(12A)-C(11A)-C(17A)	112.1(5)
C(13A)-C(12A)-C(18A)	117.5(5)
C(13A)-C(12A)-C(11A)	103.9(5)
C(18A)-C(12A)-C(11A)	117.8(6)
O(4A)-C(13A)-C(14A)	109.5(5)
O(4A)-C(13A)-C(12A)	115.0(6)
C(14A)-C(13A)-C(12A)	104.0(5)
O(3A)-C(14A)-C(1A)	127.9(6)
O(3A)-C(14A)-C(13A)	123.9(6)
C(1A)-C(14A)-C(13A)	108.1(6)
O(2A)-C(15A)-C(4A)	111.0(5)
C(20A)-C(18A)-C(12A)	110.3(6)
C(20A)-C(18A)-C(19A)	111.6(7)
C(12A)-C(18A)-C(19A)	113.5(7)
C(2B)-C(1B)-C(14B)	119.0(5)
C(2B)-C(1B)-C(11B)	132.8(5)
C(14B)-C(1B)-C(11B)	108.1(5)
C(1B)-C(2B)-C(3B)	131.8(5)
C(4B)-C(3B)-C(2B)	118.4(5)
C(4B)-C(3B)-C(8B)	123.7(5)
C(2B)-C(3B)-C(8B)	117.8(5)
C(3B)-C(4B)-C(15B)	123.0(5)
C(3B)-C(4B)-C(5B)	121.8(5)
C(15B)-C(4B)-C(5B)	115.2(5)
O(1B)-C(5B)-C(6B)	108.1(5)
O(1B)-C(5B)-C(4B)	110.0(5)
C(6B)-C(5B)-C(4B)	113.4(5)
C(5B)-C(6B)-C(7B)	110.0(5)
C(6B)-C(7B)-C(8B)	114.7(5)
C(16B)-C(8B)-C(3B)	109.8(5)
C(16B)-C(8B)-C(7B)	109.1(5)
C(3B)-C(8B)-C(7B)	110.2(5)
C(16B)-C(8B)-C(9B)	110.9(5)
C(3B)-C(8B)-C(9B)	111.7(5)
C(7B)-C(8B)-C(9B)	105.1(5)
C(10B)-C(9B)-C(8B)	118.0(6)
C(11B)-C(10B)-C(9B)	117.1(5)
C(10B)-C(11B)-C(1B)	114.5(5)
C(10B)-C(11B)-C(17B)	110.7(5)
C(1B)-C(11B)-C(17B)	107.8(5)
C(10B)-C(11B)-C(12B)	110.1(5)
C(1B)-C(11B)-C(12B)	101.3(4)
C(17B)-C(11B)-C(12B)	112.3(5)
C(13B)-C(12B)-C(11B)	105.3(5)
C(13B)-C(12B)-C(18B)	116.6(5)
C(11B)-C(12B)-C(18B)	116.6(5)
O(4B)-C(13B)-C(14B)	111.5(5)
O(4B)-C(13B)-C(12B)	112.7(5)
C(14B)-C(13B)-C(12B)	103.5(5)
O(3B)-C(14B)-C(1B)	126.5(5)
O(3B)-C(14B)-C(13B)	125.1(5)
C(1B)-C(14B)-C(13B)	108.5(5)
O(2B)-C(15B)-C(4B)	114.0(5)
C(19B)-C(18B)-C(20B)	109.6(6)
C(19B)-C(18B)-C(12B)	114.5(5)

C(20B)-C(18B)-C(12B)	111.9(5)
C(2C)-C(1C)-C(14C)	118.5(5)
C(2C)-C(1C)-C(11C)	132.7(5)
C(14C)-C(1C)-C(11C)	108.9(5)
C(1C)-C(2C)-C(3C)	131.8(5)
C(4C)-C(3C)-C(2C)	119.5(5)
C(4C)-C(3C)-C(8C)	123.3(5)
C(2C)-C(3C)-C(8C)	117.1(5)
C(3C)-C(4C)-C(5C)	122.7(6)
C(3C)-C(4C)-C(15C)	122.8(5)
C(5C)-C(4C)-C(15C)	114.5(5)
O(1C)-C(5C)-C(6C)	113.2(5)
O(1C)-C(5C)-C(4C)	108.6(5)
C(6C)-C(5C)-C(4C)	113.5(5)
C(5C)-C(6C)-C(7C)	110.3(5)
C(6C)-C(7C)-C(8C)	115.3(5)
C(9C)-C(8C)-C(3C)	115.4(5)
C(9C)-C(8C)-C(7C)	104.9(5)
C(3C)-C(8C)-C(7C)	110.3(5)
C(9C)-C(8C)-C(16C)	112.1(5)
C(3C)-C(8C)-C(16C)	105.7(5)
C(7C)-C(8C)-C(16C)	108.4(5)
C(10C)-C(9C)-C(8C)	117.8(6)
C(11C)-C(10C)-C(9C)	116.3(5)
C(1C)-C(11C)-C(10C)	113.1(5)
C(1C)-C(11C)-C(12C)	101.6(4)
C(10C)-C(11C)-C(12C)	110.5(5)
C(1C)-C(11C)-C(17C)	107.2(5)
C(10C)-C(11C)-C(17C)	111.4(5)
C(12C)-C(11C)-C(17C)	112.7(5)
C(13C)-C(12C)-C(11C)	105.9(4)
C(13C)-C(12C)-C(18C)	116.4(5)
C(11C)-C(12C)-C(18C)	116.9(5)
O(4C)-C(13C)-C(12C)	113.4(5)
O(4C)-C(13C)-C(14C)	111.3(4)
C(12C)-C(13C)-C(14C)	102.8(5)
O(3C)-C(14C)-C(1C)	127.0(6)
O(3C)-C(14C)-C(13C)	124.1(5)
C(1C)-C(14C)-C(13C)	108.9(5)
O(2C)-C(15C)-C(4C)	110.1(5)
C(20C)-C(18C)-C(19C)	108.2(6)
C(20C)-C(18C)-C(12C)	110.6(5)
C(19C)-C(18C)-C(12C)	115.3(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for guanacastepene 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)	34(3)	30(3)	23(3)	-10(3)	18(2)	-1(2)
O(2)	29(3)	32(3)	36(3)	-10(2)	16(2)	-1(2)
O(3)	46(3)	35(3)	37(3)	-5(3)	26(3)	-11(2)
O(4)	47(3)	67(4)	42(4)	-24(3)	34(3)	-32(3)
C(1)	20(3)	16(3)	20(4)	-1(3)	11(3)	-1(3)
C(2)	21(4)	24(4)	27(5)	-4(3)	11(4)	7(3)
C(3)	17(3)	23(4)	15(4)	2(3)	5(3)	-5(3)
C(4)	21(4)	25(4)	19(4)	2(3)	11(3)	-2(3)
C(5)	18(4)	28(4)	23(4)	6(3)	12(3)	16(3)
C(6)	33(4)	32(4)	23(4)	1(3)	21(4)	-3(3)
C(7)	31(4)	21(4)	31(5)	0(3)	18(4)	-2(3)
C(8)	19(3)	24(4)	12(4)	-8(3)	8(3)	-9(3)
C(9)	34(5)	21(5)	41(6)	-1(4)	26(4)	-4(4)
C(10)	34(4)	31(4)	13(4)	-11(3)	11(3)	-13(3)
C(11)	18(4)	26(4)	20(4)	4(3)	8(3)	1(3)
C(12)	21(3)	38(4)	21(4)	4(3)	8(3)	5(3)
C(13)	22(4)	32(4)	13(4)	-2(3)	7(3)	-8(3)
C(14)	32(4)	21(4)	33(5)	3(4)	20(4)	2(3)
C(15)	31(4)	26(4)	26(4)	3(3)	18(4)	-1(3)
C(16)	24(4)	29(4)	18(4)	5(3)	7(3)	15(3)
C(17)	23(4)	52(5)	20(4)	-3(3)	5(3)	-3(3)
C(18)	57(5)	47(5)	39(5)	-13(4)	35(5)	-19(4)
C(19)	67(5)	67(5)	25(5)	2(4)	20(4)	7(4)
C(20)	96(6)	37(5)	65(6)	1(4)	61(5)	0(4)
O(1A)	40(3)	51(3)	19(3)	6(2)	19(2)	-4(2)
O(2A)	49(3)	31(3)	37(3)	-10(2)	24(3)	-21(2)
O(3A)	46(3)	34(3)	45(3)	-12(3)	22(3)	4(2)
O(4A)	36(3)	92(4)	42(4)	-25(3)	25(3)	-7(3)
C(1A)	21(4)	23(4)	22(4)	0(3)	10(3)	4(3)
C(2A)	23(4)	27(4)	13(4)	-2(3)	5(3)	0(3)
C(3A)	26(4)	31(4)	22(4)	-1(3)	15(3)	-5(3)
C(4A)	25(4)	32(4)	27(4)	-2(3)	17(3)	2(3)
C(5A)	30(4)	46(5)	16(4)	-3(3)	8(3)	-8(3)
C(6A)	42(4)	33(4)	40(5)	1(3)	27(4)	3(3)
C(7A)	33(4)	25(4)	38(5)	0(3)	21(4)	-3(3)
C(8A)	30(4)	18(4)	29(5)	-11(3)	18(4)	-6(3)
C(9A)	32(4)	38(4)	32(5)	-4(4)	17(4)	-5(4)
C(10A)	33(4)	25(4)	58(5)	-2(4)	28(4)	-7(3)
C(11A)	22(3)	27(4)	24(5)	-5(3)	9(3)	-2(3)
C(12A)	26(4)	56(5)	29(5)	3(4)	14(4)	6(4)
C(13A)	29(4)	46(5)	25(5)	-11(4)	7(4)	3(3)
C(14A)	26(4)	39(5)	29(5)	-5(4)	7(4)	9(4)
C(15A)	54(5)	29(4)	29(5)	10(3)	29(4)	0(3)
C(16A)	40(4)	30(4)	41(5)	7(3)	29(4)	3(3)
C(17A)	46(4)	58(5)	22(5)	-6(4)	8(4)	6(4)
C(18A)	36(5)	79(6)	81(7)	-24(5)	39(5)	-22(4)
C(19A)	28(5)	135(8)	101(8)	-44(7)	27(5)	-13(6)
C(20A)	107(8)	124(8)	117(9)	-10(7)	92(8)	-52(7)
O(1B)	37(3)	33(3)	30(3)	2(2)	22(2)	8(2)
O(2B)	28(3)	37(3)	30(3)	2(2)	12(2)	19(2)
O(3B)	33(3)	46(3)	28(3)	9(3)	17(2)	4(2)
O(4B)	41(3)	47(3)	35(4)	-7(3)	28(3)	-14(3)
C(1B)	27(4)	16(4)	24(4)	4(3)	21(4)	-1(3)

C(2B)	34(4)	20(4)	16(4)	3(3)	11(3)	3(3)
C(3B)	28(4)	22(4)	18(4)	1(3)	14(3)	-8(3)
C(4B)	17(3)	28(4)	21(4)	-4(3)	6(3)	5(3)
C(5B)	15(3)	45(5)	22(5)	-3(4)	9(3)	1(3)
C(6B)	37(4)	26(4)	51(5)	-4(4)	31(4)	-6(3)
C(7B)	52(5)	29(4)	49(5)	6(4)	38(4)	-1(4)
C(8B)	26(4)	25(4)	25(4)	-1(3)	14(3)	4(3)
C(9B)	45(5)	27(4)	40(5)	16(4)	30(4)	4(4)
C(10B)	41(4)	20(4)	48(5)	16(3)	35(4)	12(3)
C(11B)	26(4)	23(4)	27(4)	5(3)	19(3)	6(3)
C(12B)	23(4)	29(4)	26(4)	3(3)	10(3)	-1(3)
C(13B)	24(4)	36(4)	21(4)	-2(3)	16(3)	-2(3)
C(14B)	24(4)	25(4)	15(4)	-11(3)	2(3)	-11(3)
C(15B)	35(4)	25(4)	27(5)	-5(3)	17(4)	0(3)
C(16B)	59(5)	36(4)	48(5)	-7(4)	39(4)	-10(4)
C(17B)	32(4)	39(4)	28(4)	-5(4)	14(4)	0(3)
C(18B)	29(4)	45(4)	37(5)	8(4)	22(4)	8(4)
C(19B)	27(4)	77(6)	58(6)	8(5)	24(4)	-1(4)
C(20B)	81(6)	62(6)	58(6)	7(5)	43(5)	37(5)
O(1C)	34(3)	36(3)	28(3)	12(2)	16(2)	7(2)
O(2C)	28(3)	45(3)	30(4)	19(3)	1(3)	-6(2)
O(3C)	27(3)	36(3)	25(3)	0(2)	15(2)	9(2)
O(4C)	31(3)	50(3)	35(3)	-8(3)	24(3)	-3(2)
C(1C)	21(4)	22(4)	20(4)	-6(3)	13(3)	-4(3)
C(2C)	13(3)	19(4)	23(4)	1(3)	6(3)	-2(3)
C(3C)	26(4)	25(4)	25(4)	-3(3)	14(3)	-1(3)
C(4C)	27(4)	40(5)	14(4)	-4(3)	11(3)	-15(3)
C(5C)	17(4)	43(4)	32(4)	3(3)	17(3)	-3(3)
C(6C)	55(5)	37(5)	29(5)	-13(4)	32(4)	-6(4)
C(7C)	45(4)	27(4)	45(5)	-4(4)	33(4)	3(3)
C(8C)	29(4)	26(4)	23(5)	-1(3)	16(4)	1(3)
C(9C)	66(6)	25(5)	54(6)	5(4)	51(5)	15(4)
C(10C)	48(4)	33(4)	29(5)	16(4)	24(4)	18(3)
C(11C)	30(4)	20(4)	26(4)	5(3)	19(4)	4(3)
C(12C)	34(4)	15(3)	20(4)	4(3)	11(3)	0(3)
C(13C)	20(4)	25(4)	14(4)	3(3)	8(3)	-1(3)
C(14C)	10(3)	28(4)	13(4)	-1(3)	0(3)	-2(3)
C(15C)	26(4)	25(4)	26(5)	-1(3)	12(4)	-2(3)
C(16C)	55(5)	32(4)	57(6)	-12(4)	39(5)	-10(4)
C(17C)	13(3)	45(4)	44(5)	13(4)	8(3)	4(3)
C(18C)	30(4)	27(4)	40(5)	7(4)	17(4)	3(3)
C(19C)	48(5)	66(5)	30(5)	12(4)	18(4)	9(4)
C(20C)	80(6)	60(6)	50(6)	22(4)	31(5)	-13(5)
O(2W)	43(3)	66(4)	34(4)	-13(4)	26(3)	-7(3)
O(1W)	51(3)	69(4)	45(4)	-13(3)	38(3)	-21(3)

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

	x	y	z	U(eq)
H(2B)	11766	8571	4810	29
H(5A)	11049	8078	7526	27
H(6A)	10330	7160	7200	31
H(6B)	11597	7264	7344	31
H(7A)	9502	7168	5125	32
H(7B)	10460	6710	5690	32
H(10A)	11810	7089	3515	31
H(10B)	10619	6931	2386	31
H(12A)	12412	7589	2459	33
H(13A)	11292	8531	1280	28
H(15A)	10786	8946	5274	31
H(15B)	10070	8909	5968	31
H(16A)	12672	7286	6477	38
H(16B)	12678	7267	5266	38
H(16C)	12293	6758	5714	38
H(17A)	9182	7859	2100	51
H(17B)	9309	7631	1034	51
H(17C)	9591	8239	1396	51
H(18A)	10719	7177	732	51
H(19A)	10294	7599	-1012	82
H(19B)	11036	8105	-310	82
H(19C)	9860	7957	-296	82
H(20A)	11978	7043	-69	85
H(20B)	12687	6980	1317	85
H(20C)	12805	7511	723	85
H(2AB)	8038	9432	779	27
H(5AA)	5294	9878	1461	39
H(6AA)	5655	10752	2426	43
H(6AB)	5426	10700	1118	43
H(7AA)	7691	10772	3136	36
H(7AB)	7070	11243	2229	36
H(10C)	9121	10968	678	43
H(10D)	10264	11138	1844	43
H(12B)	10112	10493	-38	44
H(13B)	11482	9586	1086	43
H(15C)	7579	9035	1719	40
H(15D)	7071	9055	2603	40
H(16D)	6189	10685	-57	49
H(16E)	7354	10737	-150	49
H(16F)	6895	11230	272	49
H(17D)	10743	10205	3303	68
H(17E)	11732	10474	3104	68
H(17F)	11455	9858	2845	68
H(18B)	11837	10949	1590	73
H(19D)	13644	10573	1966	135
H(19E)	12987	10049	1282	135
H(19F)	13011	10202	2472	135
H(20D)	11050	11130	-407	150
H(20E)	11801	10658	-517	150
H(20F)	12443	11166	255	150
H(2BB)	7121	9559	8166	28
H(5BA)	9569	9618	6755	33

H(6BA)	9303	10448	5784	41
H(6BB)	9476	10492	7074	41
H(7BA)	7278	10520	4989	45
H(7BB)	7912	11025	5771	45
H(10E)	5403	10997	6814	37
H(10F)	4307	10936	5543	37
H(12C)	4518	10708	7778	33
H(13C)	3479	9694	7493	30
H(15E)	7791	9014	7703	34
H(15F)	7647	8840	6473	34
H(16G)	8450	10837	8062	63
H(16H)	7181	10891	7937	63
H(16I)	7576	11288	7249	63
H(17G)	3653	9595	5755	50
H(17H)	4316	9808	5091	50
H(17I)	3174	10104	4934	50
H(18C)	2739	10824	5780	41
H(19G)	1054	10478	5694	80
H(19H)	1831	10127	6824	80
H(19I)	1861	10018	5643	80
H(20G)	1825	11282	6673	95
H(20H)	3189	11413	7285	95
H(20I)	2704	11015	7893	95
H(2CB)	4453	8471	5454	23
H(5CA)	5995	8453	3085	34
H(6CA)	6958	7620	3303	42
H(6CB)	5626	7587	3016	42
H(7CA)	7610	7469	5273	41
H(7CB)	6766	7000	4523	41
H(10G)	5454	7002	6829	42
H(10H)	6704	6943	7959	42
H(12D)	4681	7297	7944	29
H(13D)	5178	8293	9074	24
H(15G)	5044	9032	4888	31
H(15H)	6175	9209	4811	31
H(16J)	4436	7301	3843	64
H(16K)	4438	7178	5037	64
H(16L)	5067	6781	4573	64
H(17J)	7541	8065	8152	55
H(17K)	7650	7768	9275	55
H(17L)	6968	8318	8867	55
H(18D)	6639	7085	9661	39
H(19J)	6903	7442	11416	73
H(19K)	5848	7845	10721	73
H(19L)	7017	7899	10638	73
H(20J)	5650	6708	10577	96
H(20K)	4957	6607	9201	96
H(20L)	4521	7054	9761	96
H(1OC)	8090(50)	8240(20)	4990(50)	33(19)
H(1OB)	8190(50)	9210(20)	5010(50)	40(20)
H(4CO)	3540(50)	8190(20)	8830(50)	7(19)
H(1AO)	7090(80)	9630(40)	3640(80)	140(40)
H(1WB)	14890(90)	8640(40)	800(80)	150(30)
H(1O)	9460(40)	8243(18)	6980(40)	0(16)
H(4O)	13630(60)	8620(30)	2450(60)	60(30)
H(1WA)	13560(60)	8410(20)	850(60)	40(20)
H(4BO)	3600(40)	9911(19)	8980(40)	0(17)
H(9CB)	6940(40)	6880(20)	6360(50)	31(17)

H(9CA)	7550(50)	7510(20)	7100(50)	35(18)
H(9BB)	5920(40)	11030(20)	5260(40)	26(15)
H(9AB)	9360(50)	10760(20)	2950(50)	30(18)
H(9B)	10340(40)	6760(20)	3800(40)	10(16)
H(9A)	9640(60)	7300(30)	3320(60)	80(30)
H(9AA)	8620(50)	11400(20)	2080(50)	60(20)
H(2WB)	2280(40)	9254(19)	8530(50)	0(19)
H(9BA)	5510(60)	10350(30)	5080(60)	70(20)
H(2CO)	5150(70)	9380(30)	3260(70)	90(30)
H(2WA)	3140(80)	9140(40)	9790(90)	140(40)
H(2O)	13070(100)	8800(40)	7090(90)	230(50)
H(4AO)	11270(100)	9890(50)	-780(110)	290(60)

Table 1. Crystal data and structure refinement for guanacastepene D.

Identification code	sean16	
Empirical formula	C22 H27 N O3	
Formula weight	353.45	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 7.6070(8) Å	α= 90°.
	b = 9.5314(12) Å	β= 90°.
	c = 25.900(4) Å	γ = 90°.
Volume	1877.9(4) $Å^3$	
Z	4	
Density (calculated)	1.250 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	760	
Crystal size	0.40 x 0.05 x 0.02 mm^3	
Theta range for data collection	2.65 to 21.96°.	
Index ranges	-8<=h<=6, -10<=k<=10, -27<=l<=26	
Reflections collected	9384	
Independent reflections	2273 [R(int) = 0.0646]	
Completeness to theta = 21.96°	99.8 %	
Absorption correction	SADBETA	
Max. and min. transmission	0.9984 and 0.612314	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2273 / 0 / 343	
Goodness-of-fit on F^2	0.999	
Final R indices [I>2sigma(I)]	R1 = 0.0407, wR2 = 0.0733	
R indices (all data)	R1 = 0.0592, wR2 = 0.0787	
Absolute structure parameter	1.0(17)	
Largest diff. peak and hole	0.138 and -0.189 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	1425(3)	-3389(2)	8883(1)	50(1)
O(2)	4363(3)	-2644(2)	9448(1)	34(1)
O(3)	10112(3)	235(2)	9533(1)	30(1)
N(1)	7381(3)	-417(2)	9225(1)	23(1)
C(1)	4362(4)	-570(3)	8864(1)	19(1)
C(2)	5877(4)	260(3)	9008(1)	22(1)
C(3)	6207(4)	1659(3)	8970(1)	24(1)
C(4)	7956(4)	1896(3)	9185(1)	24(1)
C(5)	8664(5)	3164(4)	9251(1)	35(1)
C(6)	7701(5)	4452(4)	9083(2)	45(1)
C(7)	6264(5)	4127(4)	8692(2)	40(1)
C(8)	5029(4)	2889(3)	8845(1)	29(1)
C(9)	3794(5)	2623(4)	8390(2)	32(1)
C(10)	2504(5)	1384(3)	8444(2)	31(1)
C(11)	3244(4)	-127(3)	8399(1)	23(1)
C(12)	1673(4)	-1178(3)	8410(1)	25(1)
C(13)	2190(4)	-2286(4)	8792(1)	31(1)
C(14)	3789(4)	-1795(3)	9059(1)	27(1)
C(15)	8670(5)	526(3)	9346(1)	24(1)
C(16)	3987(5)	3287(4)	9333(2)	38(1)
C(17)	4363(5)	-262(4)	7907(2)	34(1)
C(18)	867(5)	-1704(4)	7896(1)	34(1)
C(19)	-1109(6)	-1979(5)	7958(2)	50(1)
C(20)	1742(6)	-3009(6)	7676(2)	54(1)
C(21)	7434(5)	-1896(3)	9369(1)	27(1)
C(22)	5932(5)	-2265(4)	9724(1)	31(1)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene D.

O(1)-C(13)	1.224(4)
O(2)-C(14)	1.364(3)
O(2)-C(22)	1.438(4)
O(3)-C(15)	1.231(4)
N(1)-C(15)	1.366(4)
N(1)-C(2)	1.428(4)
N(1)-C(21)	1.459(4)
C(1)-C(14)	1.345(4)
C(1)-C(2)	1.448(4)
C(1)-C(11)	1.533(4)
C(2)-C(3)	1.361(4)
C(3)-C(4)	1.459(4)
C(3)-C(8)	1.511(4)
C(4)-C(5)	1.334(4)
C(4)-C(15)	1.475(5)
C(5)-C(6)	1.494(5)
C(6)-C(7)	1.522(5)
C(7)-C(8)	1.560(5)
C(8)-C(9)	1.529(5)
C(8)-C(16)	1.538(5)
C(9)-C(10)	1.542(5)
C(10)-C(11)	1.551(4)
C(11)-C(17)	1.538(5)
C(11)-C(12)	1.560(4)
C(12)-C(13)	1.500(5)
C(12)-C(18)	1.548(5)
C(13)-C(14)	1.476(4)
C(18)-C(19)	1.534(5)
C(18)-C(20)	1.521(6)
C(21)-C(22)	1.509(5)
C(14)-O(2)-C(22)	119.0(3)
C(15)-N(1)-C(2)	111.6(2)
C(15)-N(1)-C(21)	123.9(3)
C(2)-N(1)-C(21)	124.0(3)
C(14)-C(1)-C(2)	129.4(3)
C(14)-C(1)-C(11)	110.8(3)
C(2)-C(1)-C(11)	119.6(3)
C(3)-C(2)-N(1)	108.8(3)
C(3)-C(2)-C(1)	131.6(3)
N(1)-C(2)-C(1)	119.5(2)
C(2)-C(3)-C(4)	107.0(3)
C(2)-C(3)-C(8)	131.8(3)
C(4)-C(3)-C(8)	120.2(3)
C(5)-C(4)-C(3)	123.9(3)
C(5)-C(4)-C(15)	128.1(3)
C(3)-C(4)-C(15)	107.8(3)
C(4)-C(5)-C(6)	120.6(3)
C(5)-C(6)-C(7)	112.2(3)
C(6)-C(7)-C(8)	114.6(3)
C(3)-C(8)-C(9)	113.7(3)
C(3)-C(8)-C(16)	108.7(3)
C(9)-C(8)-C(16)	111.0(3)
C(3)-C(8)-C(7)	106.5(3)
C(9)-C(8)-C(7)	107.4(3)
C(16)-C(8)-C(7)	109.4(3)

C(8)-C(9)-C(10)	116.6(3)
C(9)-C(10)-C(11)	118.2(3)
C(1)-C(11)-C(10)	113.5(3)
C(1)-C(11)-C(17)	108.7(3)
C(10)-C(11)-C(17)	110.0(3)
C(1)-C(11)-C(12)	103.5(2)
C(10)-C(11)-C(12)	108.4(3)
C(17)-C(11)-C(12)	112.6(3)
C(13)-C(12)-C(18)	116.3(3)
C(13)-C(12)-C(11)	105.2(3)
C(18)-C(12)-C(11)	119.8(3)
O(1)-C(13)-C(14)	125.0(3)
O(1)-C(13)-C(12)	127.4(3)
C(14)-C(13)-C(12)	107.6(3)
C(1)-C(14)-O(2)	133.6(3)
C(1)-C(14)-C(13)	111.5(3)
O(2)-C(14)-C(13)	115.0(3)
O(3)-C(15)-N(1)	125.6(3)
O(3)-C(15)-C(4)	129.7(3)
N(1)-C(15)-C(4)	104.7(3)
C(19)-C(18)-C(20)	109.1(4)
C(19)-C(18)-C(12)	110.7(3)
C(20)-C(18)-C(12)	114.4(4)
N(1)-C(21)-C(22)	111.1(3)
O(2)-C(22)-C(21)	112.5(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for guanacastepene D. 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)	46(2)	43(2)	62(2)	12(1)	-14(1)	-25(1)
O(2)	33(2)	33(1)	35(2)	12(1)	-6(1)	-10(1)
O(3)	22(2)	37(1)	32(1)	-3(1)	-3(1)	0(1)
N(1)	24(2)	18(2)	25(2)	3(1)	-3(1)	0(1)
C(1)	18(2)	23(2)	17(2)	-2(2)	1(2)	1(2)
C(2)	23(2)	25(2)	18(2)	1(2)	-1(2)	2(2)
C(3)	26(2)	28(2)	20(2)	1(2)	2(2)	0(2)
C(4)	25(2)	26(2)	22(2)	-2(2)	-1(2)	-1(2)
C(5)	30(2)	30(2)	44(2)	-1(2)	-4(2)	-1(2)
C(6)	42(3)	25(2)	69(3)	-1(2)	-6(3)	-6(2)
C(7)	41(3)	24(2)	56(3)	11(2)	-3(2)	1(2)
C(8)	32(2)	22(2)	32(2)	5(2)	1(2)	-1(2)
C(9)	35(2)	30(2)	33(2)	11(2)	-4(2)	3(2)
C(10)	28(2)	36(2)	29(2)	3(2)	-10(2)	7(2)
C(11)	23(2)	25(2)	22(2)	-2(2)	-3(2)	0(2)
C(12)	20(2)	31(2)	24(2)	-9(2)	2(2)	2(2)
C(13)	29(2)	36(2)	29(2)	-6(2)	-1(2)	-6(2)
C(14)	32(2)	24(2)	23(2)	3(2)	-1(2)	3(2)
C(15)	22(2)	32(2)	18(2)	-2(2)	5(2)	0(2)
C(16)	36(2)	39(2)	37(2)	-9(2)	-2(2)	5(2)
C(17)	30(3)	43(3)	28(2)	-1(2)	2(2)	-3(2)
C(18)	23(2)	49(2)	29(2)	-8(2)	0(2)	-5(2)
C(19)	35(3)	74(3)	42(3)	-19(3)	-7(2)	-4(2)
C(20)	39(3)	66(3)	57(4)	-33(3)	5(2)	-11(3)
C(21)	23(2)	26(2)	33(2)	10(2)	-2(2)	1(2)
C(22)	31(2)	28(2)	32(2)	6(2)	-7(2)	-3(2)

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

	x	y	z	U(eq)
H(5)	9760(50)	3240(30)	9404(12)	39(10)
H(6B)	8550(40)	5190(30)	8931(11)	42(10)
H(6A)	7200(50)	4960(40)	9418(14)	68(13)
H(7B)	5570(40)	4990(30)	8657(11)	37(10)
H(7A)	6790(50)	3840(40)	8357(16)	62(13)
H(9B)	4440(40)	2560(30)	8046(13)	47(11)
H(9A)	3000(40)	3510(30)	8347(13)	50(10)
H(10B)	1850(40)	1480(30)	8777(14)	40(11)
H(10A)	1550(40)	1480(30)	8158(13)	32(9)
H(12)	770(30)	-650(20)	8577(9)	6(7)
H(16C)	3170(50)	2450(40)	9456(12)	49(11)
H(16B)	4820(50)	3490(30)	9625(14)	60(12)
H(16A)	3160(50)	4190(40)	9254(15)	79(13)
H(17C)	4830(40)	-1200(30)	7851(11)	30(9)
H(17B)	5390(40)	310(30)	7942(11)	26(9)
H(17A)	3760(50)	50(40)	7593(15)	69(13)
H(18)	1040(40)	-950(30)	7641(11)	29(9)
H(19C)	-1720(50)	-2160(40)	7593(15)	70(13)
H(19B)	-1280(50)	-2880(40)	8233(17)	89(14)
H(19A)	-1550(40)	-1120(30)	8084(13)	37(11)
H(20C)	2970(50)	-2900(40)	7678(13)	43(12)
H(20B)	1520(50)	-3960(40)	7899(16)	83(15)
H(20A)	1440(50)	-3220(40)	7334(15)	54(13)
H(21B)	8630(40)	-2050(30)	9538(11)	36(9)
H(21A)	7340(40)	-2490(30)	9025(12)	22(8)
H(22B)	5640(30)	-1420(30)	9949(10)	15(8)
H(22A)	6220(30)	-3110(30)	9925(10)	15(7)

Table 1. Crystal data and structure refinement for guanacastepene E.

Identification code	shana2	
Empirical formula	C44 H64 O10	
Formula weight	752.95	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 9.7574(4) Å	α= 90°.
	b = 17.5875(8) Å	β= 93.7310(10)°.
	c = 11.7967(5) Å	γ = 90°.
Volume	2020.12(15) $Å^3$	
Z	2	
Density (calculated)	1.238 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	816	
Crystal size	0.1 x 0.2 x 0.3 mm^3	
Theta range for data collection	1.73 to 25.71°.	
Index ranges	-11<=h<=11, -20<=k<=21, -8<=l<=14	
Reflections collected	9619	
Independent reflections	6263 [R(int) = 0.0439]	
Absorption correction	SADABS	
Max. and min. transmission	1 and 0.715029	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5567 / 1 / 488	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0522, wR2 = 0.1209	
R indices (all data)	R1 = 0.0804, wR2 = 0.1450	
Absolute structure parameter	0.28(128)	
Extinction coefficient	0.0102(12)	
Largest diff. peak and hole	0.286 and -0.223 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	8134(3)	7372(2)	8148(2)	41(1)
O(2)	10777(3)	8231(2)	5532(2)	38(1)
O(3)	8827(3)	8735(2)	3485(2)	41(1)
O(4)	9468(3)	8177(1)	1368(2)	28(1)
O(5)	11038(3)	9022(2)	812(3)	49(1)
C(1)	10286(4)	8259(2)	6653(3)	31(1)
C(2)	10056(4)	7443(2)	6957(3)	28(1)
C(3)	9564(4)	7174(2)	8065(3)	31(1)
C(4)	9780(5)	6322(2)	8185(4)	35(1)
C(5)	9336(4)	5904(2)	7088(3)	31(1)
C(6)	10160(4)	6137(2)	6073(3)	25(1)
C(7)	9384(4)	5848(2)	4974(3)	28(1)
C(8)	10017(4)	6038(2)	3842(3)	28(1)
C(9)	9541(4)	6791(2)	3269(3)	26(1)
C(10)	10611(4)	7107(2)	2450(3)	26(1)
C(11)	10314(4)	7971(2)	2375(3)	26(1)
C(12)	9459(4)	8146(2)	3394(3)	30(1)
C(13)	9438(4)	7454(2)	4144(3)	26(1)
C(14)	10622(4)	7479(2)	5081(3)	29(1)
C(15)	10283(4)	6995(2)	6084(3)	25(1)
C(16)	11584(4)	5774(3)	6192(4)	34(1)
C(17)	8119(4)	6689(2)	2649(4)	32(1)
C(18)	10759(4)	6748(2)	1288(3)	26(1)
C(19)	12019(4)	7086(2)	759(3)	33(1)
C(20)	10933(5)	5875(2)	1304(4)	37(1)
C(21)	9903(4)	8731(2)	690(3)	32(1)
C(22)	8832(4)	8920(2)	-229(4)	39(1)
O(1')	2803(3)	8679(2)	-1314(2)	48(1)
O(2')	5985(3)	8122(2)	1364(2)	37(1)
O(3')	4416(4)	7398(2)	3303(3)	50(1)
O(4')	4779(3)	8036(2)	5473(2)	29(1)
O(5')	6470(3)	7211(2)	6023(3)	40(1)
C(1')	5408(4)	8038(2)	221(4)	32(1)
C(2')	4866(4)	8806(2)	-98(3)	28(1)
C(3')	4147(4)	9016(2)	-1213(4)	35(1)
C(4')	4085(5)	9879(2)	-1354(4)	36(1)
C(5')	3615(4)	10259(2)	-271(3)	32(1)
C(6')	4569(4)	10099(2)	794(3)	24(1)
C(7')	3774(4)	10305(2)	1845(3)	26(1)
C(8')	4521(4)	10174(2)	3004(3)	26(1)
C(9')	4342(4)	9382(2)	3556(3)	23(1)
C(10')	5495(4)	9206(2)	4504(3)	26(1)
C(11')	5552(4)	8329(2)	4555(3)	28(1)
C(12')	4807(4)	8052(2)	3456(3)	31(1)
C(13')	4482(4)	8721(2)	2687(3)	24(1)
C(14')	5594(4)	8839(2)	1818(3)	27(1)
C(15')	5002(4)	9270(2)	791(3)	24(1)
C(16')	5875(4)	10603(2)	758(4)	34(1)
C(17')	2920(4)	9313(2)	4031(4)	30(1)
C(18')	5442(4)	9574(2)	5689(3)	30(1)
C(19')	6761(4)	9371(3)	6410(4)	39(1)
C(20')	5253(5)	10437(2)	5692(4)	35(1)
C(21')	5328(5)	7479(2)	6127(3)	31(1)

C(22')	4377(5)	7239(2)	7000(4)	39(1)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene E.

O(1)-C(3)	1.448(5)
O(2)-C(14)	1.429(5)
O(2)-C(1)	1.436(5)
O(3)-C(12)	1.213(5)
O(4)-C(21)	1.345(5)
O(4)-C(11)	1.448(5)
O(5)-C(21)	1.220(5)
C(1)-C(2)	1.499(6)
C(2)-C(15)	1.327(5)
C(2)-C(3)	1.498(6)
C(3)-C(4)	1.518(6)
C(4)-C(5)	1.526(6)
C(5)-C(6)	1.540(5)
C(6)-C(15)	1.514(6)
C(6)-C(16)	1.528(6)
C(6)-C(7)	1.544(5)
C(7)-C(8)	1.544(5)
C(8)-C(9)	1.544(5)
C(9)-C(17)	1.535(5)
C(9)-C(13)	1.565(6)
C(9)-C(10)	1.570(5)
C(10)-C(18)	1.525(5)
C(10)-C(11)	1.549(5)
C(11)-C(12)	1.539(6)
C(12)-C(13)	1.506(6)
C(13)-C(14)	1.547(5)
C(14)-C(15)	1.511(6)
C(18)-C(19)	1.535(6)
C(18)-C(20)	1.543(6)
C(21)-C(22)	1.494(6)
O(1')-C(3')	1.437(5)
O(2')-C(14')	1.431(5)
O(2')-C(1')	1.434(5)
O(3')-C(12')	1.220(5)
O(4')-C(21')	1.337(5)
O(4')-C(11')	1.454(4)
O(5')-C(21')	1.223(5)
C(1')-C(2')	1.490(6)
C(2')-C(15')	1.329(5)
C(2')-C(3')	1.496(6)
C(3')-C(4')	1.528(6)
C(4')-C(5')	1.538(6)
C(5')-C(6')	1.539(6)
C(6')-C(15')	1.518(6)
C(6')-C(7')	1.547(5)
C(6')-C(16')	1.555(6)
C(7')-C(8')	1.525(6)
C(8')-C(9')	1.551(5)
C(9')-C(17')	1.535(5)
C(9')-C(13')	1.563(5)
C(9')-C(10')	1.565(5)
C(10')-C(11')	1.545(6)
C(10')-C(18')	1.544(5)
C(11')-C(12')	1.525(6)
C(12')-C(13')	1.507(6)
C(13')-C(14')	1.555(5)

C(14')-C(15')	1.512(5)
C(18')-C(20')	1.529(6)
C(18')-C(19')	1.537(6)
C(21')-C(22')	1.491(6)

C(14)-O(2)-C(1)	110.0(3)
C(21)-O(4)-C(11)	118.9(3)
O(2)-C(1)-C(2)	104.6(3)
C(15)-C(2)-C(3)	124.6(4)
C(15)-C(2)-C(1)	110.3(3)
C(3)-C(2)-C(1)	125.0(4)
O(1)-C(3)-C(2)	110.4(3)
O(1)-C(3)-C(4)	111.1(3)
C(2)-C(3)-C(4)	110.1(3)
C(3)-C(4)-C(5)	111.4(3)
C(4)-C(5)-C(6)	113.5(3)
C(15)-C(6)-C(16)	110.1(3)
C(15)-C(6)-C(5)	107.7(3)
C(16)-C(6)-C(5)	109.6(3)
C(15)-C(6)-C(7)	111.7(3)
C(16)-C(6)-C(7)	109.5(3)
C(5)-C(6)-C(7)	108.3(3)
C(6)-C(7)-C(8)	116.9(3)
C(9)-C(8)-C(7)	116.0(3)
C(17)-C(9)-C(8)	110.2(3)
C(17)-C(9)-C(13)	107.8(3)
C(8)-C(9)-C(13)	112.4(3)
C(17)-C(9)-C(10)	111.4(3)
C(8)-C(9)-C(10)	112.3(3)
C(13)-C(9)-C(10)	102.5(3)
C(18)-C(10)-C(11)	112.5(3)
C(18)-C(10)-C(9)	120.8(3)
C(11)-C(10)-C(9)	104.7(3)
O(4)-C(11)-C(12)	106.4(3)
O(4)-C(11)-C(10)	112.8(3)
C(12)-C(11)-C(10)	105.1(3)
O(3)-C(12)-C(13)	127.7(4)
O(3)-C(12)-C(11)	123.0(4)
C(13)-C(12)-C(11)	109.0(3)
C(12)-C(13)-C(14)	110.9(3)
C(12)-C(13)-C(9)	102.2(3)
C(14)-C(13)-C(9)	114.6(3)
O(2)-C(14)-C(15)	104.7(3)
O(2)-C(14)-C(13)	110.4(3)
C(15)-C(14)-C(13)	110.6(3)
C(2)-C(15)-C(14)	109.2(3)
C(2)-C(15)-C(6)	125.5(4)
C(14)-C(15)-C(6)	125.2(3)
C(10)-C(18)-C(19)	109.3(3)
C(10)-C(18)-C(20)	114.7(3)
C(19)-C(18)-C(20)	107.5(3)
O(5)-C(21)-O(4)	123.6(4)
O(5)-C(21)-C(22)	125.3(4)
O(4)-C(21)-C(22)	111.1(4)
C(14')-O(2')-C(1')	110.2(3)
C(21')-O(4')-C(11')	118.8(3)
O(2')-C(1')-C(2')	104.8(3)
C(15')-C(2')-C(1')	110.0(3)

C(15')-C(2')-C(3')	124.0(4)
C(1')-C(2')-C(3')	125.8(4)
O(1')-C(3')-C(2')	110.1(3)
O(1')-C(3')-C(4')	111.8(4)
C(2')-C(3')-C(4')	110.8(4)
C(3')-C(4')-C(5')	110.6(4)
C(4')-C(5')-C(6')	113.7(3)
C(15')-C(6')-C(5')	109.1(3)
C(15')-C(6')-C(7')	112.4(3)
C(5')-C(6')-C(7')	107.7(3)
C(15')-C(6')-C(16')	108.6(3)
C(5')-C(6')-C(16')	109.1(3)
C(7')-C(6')-C(16')	110.0(3)
C(8')-C(7')-C(6')	116.7(3)
C(7')-C(8')-C(9')	116.9(3)
C(17')-C(9')-C(8')	110.7(3)
C(17')-C(9')-C(13')	107.5(3)
C(8')-C(9')-C(13')	112.1(3)
C(17')-C(9')-C(10')	110.4(3)
C(8')-C(9')-C(10')	112.5(3)
C(13')-C(9')-C(10')	103.4(3)
C(11')-C(10')-C(18')	112.7(3)
C(11')-C(10')-C(9')	104.4(3)
C(18')-C(10')-C(9')	120.0(3)
O(4')-C(11')-C(12')	106.2(3)
O(4')-C(11')-C(10')	111.3(3)
C(12')-C(11')-C(10')	105.8(3)
O(3')-C(12')-C(13')	126.5(4)
O(3')-C(12')-C(11')	123.6(4)
C(13')-C(12')-C(11')	109.4(3)
C(12')-C(13')-C(14')	111.9(3)
C(12')-C(13')-C(9')	102.1(3)
C(14')-C(13')-C(9')	115.3(3)
O(2')-C(14')-C(15')	103.9(3)
O(2')-C(14')-C(13')	110.1(3)
C(15')-C(14')-C(13')	110.4(3)
C(2')-C(15')-C(14')	109.7(3)
C(2')-C(15')-C(6')	125.4(4)
C(14')-C(15')-C(6')	124.9(3)
C(20')-C(18')-C(19')	109.0(4)
C(20')-C(18')-C(10')	115.4(3)
C(19')-C(18')-C(10')	109.1(3)
O(5')-C(21')-O(4')	123.9(4)
O(5')-C(21')-C(22')	124.9(4)
O(4')-C(21')-C(22')	111.2(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for guanacastepene E. 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)	36(2)	51(2)	36(2)	1(2)	9(1)	7(2)
O(2)	55(2)	28(2)	32(2)	-8(1)	10(2)	-18(1)
O(3)	56(2)	22(2)	47(2)	3(1)	17(2)	12(2)
O(4)	32(2)	23(2)	31(2)	7(1)	1(1)	-2(1)
O(5)	45(2)	45(2)	56(2)	17(2)	0(2)	-16(2)
C(1)	37(2)	30(2)	27(2)	-5(2)	2(2)	-3(2)
C(2)	25(2)	28(2)	31(2)	0(2)	-4(2)	0(2)
C(3)	25(2)	43(3)	24(2)	-3(2)	0(2)	-2(2)
C(4)	36(2)	38(3)	30(2)	5(2)	0(2)	-6(2)
C(5)	31(2)	31(2)	31(2)	2(2)	5(2)	-7(2)
C(6)	25(2)	25(2)	26(2)	1(2)	3(2)	-2(2)
C(7)	32(2)	23(2)	31(2)	0(2)	8(2)	-3(2)
C(8)	31(2)	26(2)	26(2)	0(2)	4(2)	-1(2)
C(9)	25(2)	23(2)	30(2)	-1(2)	2(2)	-6(2)
C(10)	25(2)	23(2)	28(2)	1(2)	-1(2)	-1(2)
C(11)	28(2)	21(2)	28(2)	5(2)	1(2)	1(2)
C(12)	33(2)	26(2)	30(2)	0(2)	0(2)	-4(2)
C(13)	24(2)	24(2)	28(2)	-2(2)	5(2)	-1(2)
C(14)	30(2)	24(2)	33(2)	-5(2)	3(2)	-5(2)
C(15)	20(2)	27(2)	27(2)	1(2)	1(2)	-3(2)
C(16)	26(2)	36(3)	41(3)	2(2)	2(2)	3(2)
C(17)	29(2)	31(2)	37(2)	1(2)	-2(2)	-5(2)
C(18)	31(2)	19(2)	28(2)	1(2)	2(2)	0(2)
C(19)	35(2)	33(2)	32(2)	-2(2)	10(2)	4(2)
C(20)	49(3)	27(2)	36(3)	-1(2)	12(2)	6(2)
C(21)	42(3)	22(2)	31(2)	0(2)	6(2)	3(2)
C(22)	44(3)	29(3)	43(3)	6(2)	3(2)	6(2)
O(1')	55(2)	52(2)	35(2)	4(2)	-9(2)	-21(2)
O(2')	46(2)	31(2)	36(2)	-5(1)	4(1)	14(1)
O(3')	77(2)	25(2)	47(2)	5(2)	-8(2)	-6(2)
O(4')	32(2)	26(2)	29(2)	8(1)	3(1)	5(1)
O(5')	36(2)	38(2)	47(2)	10(2)	0(1)	8(1)
C(1')	34(2)	28(2)	33(2)	-8(2)	8(2)	-4(2)
C(2')	29(2)	29(2)	27(2)	-4(2)	10(2)	-1(2)
C(3')	42(3)	39(3)	26(2)	-3(2)	6(2)	-9(2)
C(4')	44(3)	39(3)	26(2)	4(2)	6(2)	1(2)
C(5')	36(2)	31(2)	31(2)	7(2)	1(2)	5(2)
C(6')	28(2)	20(2)	25(2)	2(2)	5(2)	3(2)
C(7')	27(2)	26(2)	26(2)	3(2)	2(2)	1(2)
C(8')	27(2)	22(2)	31(2)	1(2)	6(2)	1(2)
C(9')	25(2)	22(2)	23(2)	1(2)	3(2)	0(2)
C(10')	25(2)	25(2)	29(2)	4(2)	8(2)	-4(2)
C(11')	28(2)	32(2)	26(2)	6(2)	5(2)	1(2)
C(12')	36(2)	27(3)	32(2)	-4(2)	8(2)	3(2)
C(13')	23(2)	22(2)	26(2)	-2(2)	1(2)	2(2)
C(14')	27(2)	26(2)	29(2)	-6(2)	5(2)	3(2)
C(15')	20(2)	26(2)	27(2)	2(2)	7(2)	-1(2)
C(16')	39(3)	29(2)	36(2)	-3(2)	12(2)	-7(2)
C(17')	28(2)	28(2)	34(2)	7(2)	5(2)	-1(2)
C(18')	32(2)	30(2)	28(2)	-3(2)	4(2)	-6(2)
C(19')	37(2)	41(3)	37(3)	2(2)	-3(2)	-2(2)
C(20')	42(3)	32(3)	33(3)	-2(2)	10(2)	-2(2)
C(21')	39(3)	25(2)	28(2)	-1(2)	-5(2)	-7(2)

C(22')	60(3)	24(2)	35(3)	4(2)	7(2)	-3(2)

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

	x	y	z	U(eq)
H(1A)	7844(3)	7602(2)	7556(2)	61
H(1B)	9419(4)	8552(2)	6654(3)	38
H(1C)	10975(4)	8497(2)	7195(3)	38
H(3A)	10117(4)	7433(2)	8695(3)	37
H(4A)	9244(5)	6129(2)	8809(4)	42
H(4B)	10763(5)	6218(2)	8386(4)	42
H(5A)	8350(4)	6006(2)	6898(3)	37
H(5B)	9443(4)	5351(2)	7215(3)	37
H(7A)	8442(4)	6059(2)	4944(3)	34
H(7B)	9302(4)	5288(2)	5029(3)	34
H(8A)	11028(4)	6056(2)	3981(3)	33
H(8B)	9801(4)	5617(2)	3302(3)	33
H(10A)	11530(4)	7056(2)	2870(3)	31
H(11A)	11189(4)	8269(2)	2423(3)	31
H(13A)	8538(4)	7424(2)	4501(3)	31
H(14A)	11499(4)	7305(2)	4772(3)	35
H(16A)	11493(4)	5220(3)	6185(4)	52
H(16B)	12058(4)	5936(3)	6910(4)	52
H(16C)	12116(4)	5935(3)	5557(4)	52
H(17A)	7826(4)	7170(2)	2292(4)	48
H(17B)	7456(4)	6537(2)	3196(4)	48
H(17C)	8168(4)	6296(2)	2065(4)	48
H(18A)	9924(4)	6876(2)	787(3)	31
H(19A)	12117(4)	6856(2)	12(3)	50
H(19B)	12844(4)	6981(2)	1253(3)	50
H(19C)	11901(4)	7637(2)	674(3)	50
H(20A)	11025(5)	5691(2)	529(4)	55
H(20B)	10126(5)	5641(2)	1614(4)	55
H(20C)	11757(5)	5741(2)	1781(4)	55
H(22A)	8013(4)	8609(2)	-138(4)	58
H(22B)	9190(4)	8816(2)	-970(4)	58
H(22C)	8591(4)	9459(2)	-181(4)	58
H(1'A)	2675(3)	8426(2)	-727(2)	72
H(1'B)	4661(4)	7656(2)	183(4)	38
H(1'C)	6120(4)	7878(2)	-291(4)	38
H(3'A)	4689(4)	8805(2)	-1831(4)	42
H(4'A)	3436(5)	10010(2)	-2005(4)	44
H(4'B)	5004(5)	10074(2)	-1517(4)	44
H(5'A)	2680(4)	10077(2)	-134(3)	39
H(5'B)	3562(4)	10815(2)	-394(3)	39
H(7'A)	3516(4)	10849(2)	1789(3)	32
H(7'B)	2913(4)	10007(2)	1810(3)	32
H(8'A)	4205(4)	10564(2)	3533(3)	32
H(8'B)	5514(4)	10259(2)	2930(3)	32
H(10B)	6378(4)	9375(2)	4200(3)	31
H(11B)	6523(4)	8143(2)	4622(3)	34
H(13B)	3573(4)	8635(2)	2265(3)	28
H(14B)	6412(4)	9109(2)	2179(3)	33
H(16D)	5610(4)	11141(2)	758(4)	52
H(16E)	6343(4)	10490(2)	68(4)	52
H(16F)	6494(4)	10497(2)	1427(4)	52
H(17D)	2826(4)	8810(2)	4375(4)	45

H(17E)	2208(4)	9379(2)	3413(4)	45
H(17F)	2817(4)	9707(2)	4607(4)	45
H(18B)	4651(4)	9344(2)	6065(3)	36
H(19D)	6890(4)	8818(3)	6410(4)	58
H(19E)	6684(4)	9548(3)	7190(4)	58
H(19F)	7549(4)	9617(3)	6088(4)	58
H(20D)	4413(5)	10570(2)	5235(4)	53
H(20E)	6044(5)	10680(2)	5369(4)	53
H(20F)	5182(5)	10614(2)	6473(4)	53
H(22D)	3528(5)	7537(2)	6908(4)	59
H(22E)	4816(5)	7327(2)	7760(4)	59
H(22F)	4163(5)	6698(2)	6906(4)	59

Table 1. Crystal data and structure refinement for p-bromobenzoyl guanacastepene E.

Identification code	sean_april9	
Empirical formula	C58 H68 Br2 O12	
Formula weight	1116.94	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 7.8940(7) Å	α= 90°.
	b = 29.101(3) Å	β= 92.717(3)°.
	c = 11.6708(10) Å	γ = 90°.
Volume	2678.0(4) $Å^3$	
Z	2	
Density (calculated)	1.385 Mg/m^3	
Absorption coefficient	1.576 mm^{-1}	
F(000)	1164	
Crystal size	0.30 x 0.10 x 0.05 mm^3	
Theta range for data collection	1.75 to 24.71°.	
Index ranges	-9<=h<=9, -34<=k<=34, -13<=l<=13	
Reflections collected	23646	
Independent reflections	9058 [R(int) = 0.0566]	
Completeness to theta = 24.71°	99.9 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9254 and 0.649572	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9058 / 1 / 921	
Goodness-of-fit on F^2	0.925	
Final R indices [I>2sigma(I)]	R1 = 0.0410, wR2 = 0.0650	
R indices (all data)	R1 = 0.0703, wR2 = 0.0722	
Absolute structure parameter	0.023(6)	
Largest diff. peak and hole	0.272 and -0.289 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Br(1)	4614(1)	8366(1)	9839(1)	42(1)
O(1)	7107(3)	10048(1)	2297(3)	29(1)
O(2)	4910(4)	8938(1)	4190(3)	23(1)
O(3)	5125(4)	8167(1)	4039(3)	34(1)
O(4)	6126(4)	11705(1)	3426(2)	30(1)
O(5)	8845(4)	11903(1)	3184(3)	47(1)
O(6)	7648(5)	10843(1)	3997(3)	57(1)
C(1)	5002(5)	10576(2)	3062(4)	23(1)
C(2)	5399(5)	10206(2)	2147(4)	20(1)
C(3)	4319(5)	9784(2)	2283(3)	17(1)
C(4)	5303(5)	9437(1)	2630(3)	20(1)
C(5)	4707(5)	8970(2)	2925(4)	21(1)
C(6)	2851(5)	8905(2)	2567(4)	24(1)
C(7)	1817(6)	9342(2)	2763(4)	26(1)
C(8)	2417(5)	9763(1)	2086(4)	22(1)
C(9)	1565(7)	10193(2)	2541(5)	26(1)
C(10)	2084(6)	10660(2)	2026(4)	27(1)
C(11)	3541(5)	10905(1)	2695(3)	22(1)
C(12)	4479(5)	11272(2)	1969(4)	25(1)
C(13)	6212(5)	11337(1)	2597(4)	26(1)
C(14)	6497(6)	10892(1)	3292(4)	28(1)
C(15)	7140(6)	9583(2)	2691(4)	26(1)
C(16)	1939(7)	9701(2)	804(4)	28(1)
C(17)	2852(7)	11125(2)	3775(5)	34(1)
C(18)	3637(6)	11730(2)	1621(4)	29(1)
C(19)	1902(7)	11678(2)	1000(5)	38(1)
C(20)	4829(8)	11991(2)	859(5)	38(1)
C(21)	7567(6)	11941(2)	3684(4)	32(1)
C(22)	7284(8)	12269(2)	4644(5)	36(1)
C(23)	5023(5)	8508(2)	4623(4)	22(1)
C(24)	5011(5)	8508(2)	5891(3)	23(1)
C(25)	5636(6)	8116(2)	6462(4)	28(1)
C(26)	5543(6)	8084(2)	7628(4)	30(1)
C(27)	4813(5)	8432(2)	8229(3)	27(1)
C(28)	4200(6)	8818(2)	7682(4)	30(1)
C(29)	4320(6)	8858(2)	6506(4)	28(1)
Br(1')	-38(1)	8495(1)	-4956(1)	43(1)
O(1')	2977(3)	6898(1)	2407(3)	32(1)
O(2')	-233(4)	7893(1)	669(3)	25(1)
O(3')	-561(4)	8654(1)	876(3)	32(1)
O(4')	2715(4)	5201(1)	1441(3)	29(1)
O(5')	5447(4)	5005(1)	1762(4)	56(1)
O(6')	3445(4)	6106(1)	707(3)	57(1)
C(1')	1023(5)	6270(2)	1847(4)	23(1)
C(2')	1447(5)	6664(2)	2693(4)	24(1)
C(3')	94(5)	7028(2)	2640(4)	20(1)
C(4')	726(5)	7407(1)	2181(3)	17(1)
C(5')	-236(5)	7838(2)	1931(4)	22(1)
C(6')	-2022(6)	7819(2)	2337(4)	28(1)
C(7')	-2771(6)	7336(2)	2267(5)	28(1)
C(8')	-1713(5)	6976(2)	2947(4)	24(1)
C(9')	-2414(6)	6497(2)	2651(4)	28(1)

C(10')	-1439(6)	6077(2)	3131(4)	30(1)
C(11')	-83(5)	5883(1)	2361(4)	24(1)
C(12')	1281(6)	5577(2)	2999(4)	27(1)
C(13')	2811(6)	5583(2)	2227(4)	28(1)
C(14')	2593(5)	6018(2)	1506(4)	34(1)
C(15')	2572(6)	7346(2)	1961(5)	31(1)
C(16')	-1830(7)	7063(2)	4245(4)	30(1)
C(17')	-977(6)	5616(2)	1356(4)	34(1)
C(18')	875(6)	5091(2)	3407(4)	31(1)
C(19')	-635(9)	5069(2)	4161(6)	52(2)
C(20')	2410(8)	4883(2)	4041(5)	46(2)
C(21')	4116(6)	4952(2)	1271(4)	32(1)
C(22')	3679(7)	4586(2)	388(5)	35(1)
C(23')	-378(5)	8328(2)	276(4)	28(1)
C(24')	-243(5)	8349(2)	-998(4)	24(1)
C(25')	-317(6)	8778(2)	-1515(5)	29(1)
C(26')	-253(6)	8822(2)	-2681(5)	33(1)
C(27')	-94(4)	8432(2)	-3330(3)	30(1)
C(28')	20(6)	7995(2)	-2870(4)	30(1)
C(29')	-64(6)	7964(2)	-1676(5)	30(1)

Table 3. Bond lengths [Å] and angles [°] for p-bromobenzoyl guanacastepene E.

Br(1)-C(27)	1.903(4)
O(1)-C(15)	1.428(6)
O(1)-C(2)	1.428(5)
O(2)-C(23)	1.349(5)
O(2)-C(5)	1.480(5)
O(3)-C(23)	1.209(5)
O(4)-C(21)	1.351(5)
O(4)-C(13)	1.447(5)
O(5)-C(21)	1.195(5)
O(6)-C(14)	1.204(5)
C(1)-C(14)	1.509(6)
C(1)-C(11)	1.543(6)
C(1)-C(2)	1.559(6)
C(2)-C(3)	1.508(6)
C(3)-C(4)	1.325(6)
C(3)-C(8)	1.510(5)
C(4)-C(5)	1.484(6)
C(4)-C(15)	1.510(6)
C(5)-C(6)	1.517(6)
C(6)-C(7)	1.533(6)
C(7)-C(8)	1.546(6)
C(8)-C(9)	1.527(6)
C(8)-C(16)	1.536(6)
C(9)-C(10)	1.548(7)
C(10)-C(11)	1.535(6)
C(11)-C(17)	1.535(6)
C(11)-C(12)	1.571(6)
C(12)-C(18)	1.535(6)
C(12)-C(13)	1.533(6)
C(13)-C(14)	1.540(6)
C(18)-C(20)	1.528(7)
C(18)-C(19)	1.527(7)
C(21)-C(22)	1.497(7)
C(23)-C(24)	1.481(6)
C(24)-C(29)	1.373(6)
C(24)-C(25)	1.398(6)
C(25)-C(26)	1.369(7)
C(26)-C(27)	1.375(6)
C(27)-C(28)	1.369(6)
C(28)-C(29)	1.385(6)
Br(1')-C(27')	1.909(4)
O(1')-C(15')	1.432(5)
O(1')-C(2')	1.440(5)
O(2')-C(23')	1.348(6)
O(2')-C(5')	1.483(5)
O(3')-C(23')	1.193(5)
O(4')-C(21')	1.345(5)
O(4')-C(13')	1.441(5)
O(5')-C(21')	1.183(5)
O(6')-C(14')	1.203(5)
C(1')-C(14')	1.510(6)
C(1')-C(2')	1.539(6)
C(1')-C(11')	1.564(5)
C(2')-C(3')	1.503(6)
C(3')-C(4')	1.333(5)
C(3')-C(8')	1.495(5)

C(4')-C(15')	1.502(6)
C(4')-C(5')	1.488(6)
C(5')-C(6')	1.509(6)
C(6')-C(7')	1.525(7)
C(7')-C(8')	1.536(7)
C(8')-C(9')	1.533(6)
C(8')-C(16')	1.543(6)
C(9')-C(10')	1.536(6)
C(10')-C(11')	1.538(6)
C(11')-C(17')	1.548(6)
C(11')-C(12')	1.559(6)
C(12')-C(18')	1.531(6)
C(12')-C(13')	1.540(6)
C(13')-C(14')	1.524(6)
C(18')-C(19')	1.516(7)
C(18')-C(20')	1.516(7)
C(21')-C(22')	1.510(7)
C(23')-C(24')	1.497(6)
C(24')-C(29')	1.384(7)
C(24')-C(25')	1.385(7)
C(25')-C(26')	1.370(7)
C(26')-C(27')	1.374(7)
C(27')-C(28')	1.381(6)
C(28')-C(29')	1.401(7)

C(15)-O(1)-C(2)	110.4(3)
C(23)-O(2)-C(5)	115.8(3)
C(21)-O(4)-C(13)	117.4(3)
C(14)-C(1)-C(11)	103.9(4)
C(14)-C(1)-C(2)	111.2(3)
C(11)-C(1)-C(2)	114.2(3)
O(1)-C(2)-C(3)	105.0(3)
O(1)-C(2)-C(1)	111.0(3)
C(3)-C(2)-C(1)	110.9(3)
C(4)-C(3)-C(8)	125.5(4)
C(4)-C(3)-C(2)	109.1(3)
C(8)-C(3)-C(2)	125.4(4)
C(3)-C(4)-C(5)	125.5(4)
C(3)-C(4)-C(15)	110.4(4)
C(5)-C(4)-C(15)	124.1(4)
O(2)-C(5)-C(4)	105.7(3)
O(2)-C(5)-C(6)	108.9(3)
C(4)-C(5)-C(6)	111.3(4)
C(5)-C(6)-C(7)	111.7(4)
C(6)-C(7)-C(8)	113.8(4)
C(3)-C(8)-C(9)	111.4(4)
C(3)-C(8)-C(16)	110.5(4)
C(9)-C(8)-C(16)	110.1(4)
C(3)-C(8)-C(7)	106.3(3)
C(9)-C(8)-C(7)	108.8(3)
C(16)-C(8)-C(7)	109.7(4)
C(8)-C(9)-C(10)	117.0(4)
C(11)-C(10)-C(9)	114.6(4)
C(17)-C(11)-C(10)	109.0(4)
C(17)-C(11)-C(1)	108.7(4)
C(10)-C(11)-C(1)	112.6(3)
C(17)-C(11)-C(12)	110.7(4)
C(10)-C(11)-C(12)	113.7(4)

C(1)-C(11)-C(12)	101.9(3)
C(18)-C(12)-C(13)	112.6(4)
C(18)-C(12)-C(11)	121.5(4)
C(13)-C(12)-C(11)	105.0(4)
O(4)-C(13)-C(14)	106.3(3)
O(4)-C(13)-C(12)	110.0(3)
C(14)-C(13)-C(12)	104.6(4)
O(6)-C(14)-C(1)	127.5(4)
O(6)-C(14)-C(13)	123.0(4)
C(1)-C(14)-C(13)	108.9(4)
O(1)-C(15)-C(4)	104.3(4)
C(20)-C(18)-C(19)	109.6(4)
C(20)-C(18)-C(12)	108.4(4)
C(19)-C(18)-C(12)	114.1(4)
O(5)-C(21)-O(4)	124.4(4)
O(5)-C(21)-C(22)	125.8(5)
O(4)-C(21)-C(22)	109.7(4)
O(3)-C(23)-O(2)	123.7(4)
O(3)-C(23)-C(24)	124.5(4)
O(2)-C(23)-C(24)	111.8(4)
C(29)-C(24)-C(25)	119.6(4)
C(29)-C(24)-C(23)	123.0(4)
C(25)-C(24)-C(23)	117.2(4)
C(26)-C(25)-C(24)	119.7(5)
C(25)-C(26)-C(27)	120.0(5)
C(28)-C(27)-C(26)	121.0(4)
C(28)-C(27)-Br(1)	120.0(3)
C(26)-C(27)-Br(1)	119.0(4)
C(27)-C(28)-C(29)	119.4(4)
C(24)-C(29)-C(28)	120.3(4)
C(15')-O(1')-C(2')	109.8(3)
C(23')-O(2')-C(5')	115.8(3)
C(21')-O(4')-C(13')	119.4(4)
C(14')-C(1')-C(2')	112.1(4)
C(14')-C(1')-C(11')	103.3(4)
C(2')-C(1')-C(11')	113.5(3)
O(1')-C(2')-C(3')	105.0(3)
O(1')-C(2')-C(1')	111.3(3)
C(3')-C(2')-C(1')	111.5(4)
C(4')-C(3')-C(8')	124.0(4)
C(4')-C(3')-C(2')	108.7(3)
C(8')-C(3')-C(2')	127.1(4)
C(3')-C(4')-C(15')	110.8(4)
C(3')-C(4')-C(5')	125.3(4)
C(15')-C(4')-C(5')	123.9(4)
O(2')-C(5')-C(4')	105.1(3)
O(2')-C(5')-C(6')	111.2(3)
C(4')-C(5')-C(6')	112.6(4)
C(5')-C(6')-C(7')	112.5(4)
C(6')-C(7')-C(8')	113.6(4)
C(3')-C(8')-C(9')	112.1(3)
C(3')-C(8')-C(7')	108.0(4)
C(9')-C(8')-C(7')	108.7(4)
C(3')-C(8')-C(16')	108.7(4)
C(9')-C(8')-C(16')	109.5(4)
C(7')-C(8')-C(16')	109.9(4)
C(8')-C(9')-C(10')	118.2(4)
C(11')-C(10')-C(9')	115.5(4)

C(10')-C(11')-C(17')	108.8(4)
C(10')-C(11')-C(1')	112.1(3)
C(17')-C(11')-C(1')	108.3(4)
C(10')-C(11')-C(12')	114.5(4)
C(17')-C(11')-C(12')	110.8(4)
C(1')-C(11')-C(12')	102.1(3)
C(18')-C(12')-C(13')	112.0(4)
C(18')-C(12')-C(11')	121.7(4)
C(13')-C(12')-C(11')	104.9(4)
O(4')-C(13')-C(14')	106.7(4)
O(4')-C(13')-C(12')	110.1(4)
C(14')-C(13')-C(12')	105.2(4)
O(6')-C(14')-C(13')	123.6(4)
O(6')-C(14')-C(1')	126.6(4)
C(13')-C(14')-C(1')	109.3(4)
O(1')-C(15')-C(4')	104.3(3)
C(19')-C(18')-C(20')	109.4(5)
C(19')-C(18')-C(12')	113.7(4)
C(20')-C(18')-C(12')	110.3(4)
O(5')-C(21')-O(4')	125.2(5)
O(5')-C(21')-C(22')	126.2(5)
O(4')-C(21')-C(22')	108.5(4)
O(3')-C(23')-O(2')	124.0(4)
O(3')-C(23')-C(24')	124.4(4)
O(2')-C(23')-C(24')	111.6(4)
C(29')-C(24')-C(25')	118.9(4)
C(29')-C(24')-C(23')	123.2(5)
C(25')-C(24')-C(23')	117.9(4)
C(26')-C(25')-C(24')	120.9(5)
C(27')-C(26')-C(25')	118.7(5)
C(26')-C(27')-C(28')	123.4(4)
C(26')-C(27')-Br(1')	118.4(4)
C(28')-C(27')-Br(1')	118.1(4)
C(27')-C(28')-C(29')	116.2(4)
C(24')-C(29')-C(28')	121.8(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for p-bromobenzoyl guanacastepene E. 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}
Br(1)	59(1)	45(1)	22(1)	5(1)	0(1)	-4(1)
O(1)	13(2)	24(2)	49(2)	8(2)	-1(1)	-2(1)
O(2)	28(2)	20(2)	21(2)	5(2)	-1(1)	3(1)
O(3)	45(2)	21(2)	35(2)	-1(2)	9(2)	2(2)
O(4)	34(2)	20(2)	35(2)	-8(1)	-1(1)	-10(1)
O(5)	38(2)	42(2)	61(2)	-11(2)	10(2)	-15(2)
O(6)	62(3)	41(2)	64(3)	14(2)	-37(2)	-15(2)
C(1)	22(3)	29(3)	17(2)	9(2)	-2(2)	-1(2)
C(2)	18(2)	22(3)	18(2)	1(2)	-1(2)	2(2)
C(3)	17(2)	22(3)	13(2)	2(2)	4(2)	-2(2)
C(4)	19(2)	26(3)	16(2)	-4(2)	5(2)	-2(2)
C(5)	27(3)	17(3)	18(2)	-1(2)	3(2)	2(2)
C(6)	30(3)	24(3)	18(2)	0(2)	0(2)	-3(2)
C(7)	16(3)	31(3)	30(3)	-5(2)	4(2)	-6(2)
C(8)	17(2)	24(3)	24(2)	4(2)	-2(2)	-2(2)
C(9)	22(3)	25(3)	29(3)	1(2)	2(2)	0(2)
C(10)	18(3)	35(3)	27(3)	-7(2)	-5(2)	7(2)
C(11)	27(2)	17(3)	23(2)	-2(2)	6(2)	-2(2)
C(12)	33(3)	23(3)	18(2)	-2(2)	6(2)	1(2)
C(13)	28(3)	19(3)	29(2)	-3(2)	2(2)	-4(2)
C(14)	34(3)	24(3)	26(3)	10(2)	-6(2)	-5(2)
C(15)	17(3)	37(3)	23(3)	0(2)	-4(2)	4(2)
C(16)	19(3)	32(3)	32(3)	2(2)	-3(2)	0(2)
C(17)	40(3)	34(3)	29(3)	-4(3)	11(3)	3(3)
C(18)	38(3)	24(3)	24(3)	-5(2)	-1(2)	8(2)
C(19)	43(3)	30(3)	39(3)	1(3)	-9(3)	16(3)
C(20)	64(4)	22(3)	29(3)	3(3)	-2(3)	5(3)
C(21)	35(3)	20(3)	40(3)	3(2)	-6(2)	-5(2)
C(22)	45(4)	27(3)	36(3)	-11(3)	-11(3)	-6(3)
C(23)	23(2)	13(3)	31(2)	6(3)	4(2)	2(2)
C(24)	23(2)	15(3)	29(2)	-1(2)	-1(2)	-6(2)
C(25)	23(3)	27(3)	33(3)	1(2)	7(2)	5(2)
C(26)	37(3)	23(3)	30(3)	14(3)	-4(2)	-3(2)
C(27)	30(2)	26(3)	24(2)	-3(2)	-1(2)	-11(2)
C(28)	38(3)	26(3)	27(3)	-6(2)	6(2)	5(2)
C(29)	30(3)	23(3)	31(3)	5(2)	-6(2)	3(2)
Br(1')	55(1)	47(1)	27(1)	5(1)	2(1)	-3(1)
O(1')	11(2)	20(2)	64(2)	5(2)	0(2)	-2(1)
O(2')	36(2)	16(2)	23(2)	2(2)	2(1)	2(1)
O(3')	49(2)	17(2)	29(2)	-3(2)	-5(2)	2(2)
O(4')	28(2)	28(2)	30(2)	-6(2)	2(2)	2(2)
O(5')	26(2)	61(3)	81(3)	-18(2)	2(2)	0(2)
O(6')	74(2)	29(2)	73(3)	13(2)	50(2)	6(2)
C(1')	25(2)	24(3)	20(2)	8(2)	2(2)	-5(2)
C(2')	20(3)	27(3)	27(3)	9(2)	-2(2)	-3(2)
C(3')	16(2)	25(3)	20(2)	-4(2)	-2(2)	0(2)
C(4')	17(2)	18(2)	17(2)	-3(2)	-4(2)	1(2)
C(5')	26(3)	19(3)	22(2)	-2(2)	-2(2)	-5(2)
C(6')	36(3)	26(3)	21(3)	2(2)	-2(2)	7(2)
C(7')	19(3)	36(3)	30(3)	-1(3)	7(2)	0(2)
C(8')	15(2)	30(3)	26(2)	-2(2)	5(2)	-4(2)
C(9')	19(3)	30(3)	37(3)	-2(2)	9(2)	-6(2)

C(10')	38(3)	26(3)	27(3)	-4(2)	10(2)	-10(2)
C(11')	29(3)	21(3)	22(2)	-6(2)	2(2)	-7(2)
C(12')	37(3)	21(3)	23(3)	-8(2)	-2(2)	-2(2)
C(13')	34(3)	21(3)	28(3)	-1(2)	2(2)	-4(2)
C(14')	41(3)	21(3)	43(3)	-2(3)	18(2)	-7(3)
C(15')	20(3)	19(3)	53(4)	4(3)	2(3)	-3(2)
C(16')	35(3)	24(3)	31(3)	4(2)	12(3)	4(3)
C(17')	42(3)	38(3)	24(3)	-8(2)	6(2)	-12(3)
C(18')	51(3)	17(3)	24(3)	-2(2)	4(2)	-3(2)
C(19')	85(5)	18(3)	56(4)	12(3)	39(4)	2(3)
C(20')	86(5)	25(3)	25(3)	4(3)	-14(3)	3(3)
C(21')	30(3)	22(3)	44(3)	6(2)	14(3)	-2(2)
C(22')	36(3)	31(3)	38(3)	-8(3)	16(3)	0(3)
C(23')	24(2)	30(3)	30(2)	-4(3)	3(2)	-2(2)
C(24')	23(2)	19(3)	30(2)	-2(3)	1(2)	2(2)
C(25')	33(3)	19(3)	35(3)	6(3)	-2(2)	1(2)
C(26')	44(3)	19(3)	36(3)	13(3)	1(3)	8(2)
C(27')	25(2)	41(3)	24(2)	6(3)	3(2)	-1(2)
C(28')	32(3)	22(3)	35(3)	10(2)	1(2)	0(2)
C(29')	34(3)	16(3)	41(3)	5(3)	8(2)	3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for p-bromobenzoyl guanacastepene E.

	x	y	z	U(eq)
H(1)	4810(40)	10409(11)	3710(30)	2(9)
H(2)	5270(40)	10314(11)	1440(30)	0(9)
H(5)	5420(50)	8715(14)	2590(40)	36(13)
H(6B)	2850(40)	8851(11)	1770(30)	3(8)
H(6A)	2450(40)	8626(14)	2960(30)	32(11)
H(7B)	820(50)	9292(13)	2550(30)	15(12)
H(7A)	1820(40)	9429(11)	3610(30)	6(9)
H(9B)	1660(40)	10190(12)	3270(30)	0(10)
H(9A)	430(50)	10141(14)	2390(40)	28(13)
H(10B)	2360(50)	10614(13)	1270(30)	15(11)
H(10A)	1120(60)	10838(14)	1960(40)	28(13)
H(12)	4680(40)	11126(12)	1390(30)	12(11)
H(13)	7200(50)	11378(15)	2060(40)	44(13)
H(15B)	7570(40)	9546(12)	3440(30)	6(10)
H(15A)	7800(50)	9405(13)	2190(40)	21(11)
H(16B)	2500(50)	9930(16)	290(40)	40(13)
H(16C)	2290(60)	9388(17)	540(40)	48(15)
H(16A)	850(40)	9711(11)	740(30)	2(10)
H(17C)	2040(50)	11338(14)	3520(30)	22(13)
H(17B)	2130(60)	10943(16)	4130(40)	36(14)
H(17A)	3810(50)	11241(14)	4310(30)	29(12)
H(18)	3470(40)	11945(12)	2330(30)	11(9)
H(19C)	2030(50)	11477(16)	390(40)	49(15)
H(19B)	1060(50)	11577(14)	1590(40)	31(12)
H(19A)	1510(50)	12008(17)	650(40)	57(15)
H(20V)	4380(40)	12223(13)	550(30)	6(11)
H(20B)	5100(50)	11780(16)	190(40)	42(14)
H(20A)	6030(50)	12072(13)	1220(30)	26(12)
H(22C)	7040(70)	12530(20)	4350(50)	70(20)
H(22B)	8410(70)	12314(17)	5050(40)	61(17)
H(22A)	6650(80)	12130(20)	5160(60)	110(30)
H(25)	6250(40)	7898(12)	6090(30)	9(10)
H(20)	6020(50)	7835(15)	7990(30)	26(12)
H(28)	3750(40)	9050(12)	8060(30)	0(9)
H(29)	3850(50)	9158(13)	6090(30)	25(11)
H(1')	530(40)	6401(12)	1190(30)	0(9)
H(2')	1740(40)	6516(12)	3520(30)	14(10)
H(5')	300(50)	8107(14)	2280(30)	27(12)
H(6D)	-1900(40)	7899(12)	3120(30)	14(10)
H(6C)	-2750(50)	8007(14)	1880(30)	23(11)
H(7D)	-2910(40)	7242(13)	1500(40)	20(11)
H(7C)	-3810(40)	7326(10)	2560(30)	0(9)
H(9D)	-2500(40)	6463(11)	1810(30)	0(9)
H(9C)	-3590(60)	6474(15)	2980(40)	50(14)
H(10C)	-910(40)	6152(11)	3820(30)	8(10)
H(10D)	-2120(60)	5809(16)	3250(40)	41(14)
H(12')	1500(50)	5751(14)	3580(40)	26(13)
H(13')	3940(50)	5596(13)	2550(30)	18(11)
H(15C)	2780(60)	7317(16)	1080(40)	49(15)
H(15D)	3260(50)	7556(13)	2330(30)	14(11)
H(16F)	-1410(50)	7410(15)	4510(30)	29(11)
H(16E)	-1200(40)	6864(12)	4640(30)	0(10)

H(16D)	-2870(50)	7016(14)	4450(40)	26(13)
H(17E)	-1460(40)	5329(13)	1650(30)	14(11)
H(17D)	-330(50)	5532(13)	840(30)	18(11)
H(18C)	580(50)	4927(14)	2750(40)	25(12)
H(19F)	-630(50)	4785(17)	4470(40)	35(13)
H(19E)	-600(50)	5314(17)	4790(40)	51(15)
H(19D)	-1760(50)	5143(13)	3810(30)	18(12)
H(20F)	2740(50)	5042(14)	4640(40)	22(12)
H(20E)	3430(60)	4809(18)	3540(40)	70(18)
H(20D)	2140(40)	4566(14)	4370(30)	24(11)
H(22F)	4670(50)	4486(14)	80(40)	37(13)
H(22E)	3280(60)	4300(20)	740(50)	72(18)
H(22D)	2740(80)	4680(20)	-200(60)	110(30)
H(25')	-320(50)	9062(14)	-1110(30)	26(12)
H(26')	-420(40)	9066(13)	-3010(30)	0(10)
H(29')	-60(50)	7693(16)	-1410(40)	27(13)

Table 1. Crystal data and structure refinement for guanacastepene F.

Identification code	sean22	
Empirical formula	C66 H90 O18	
Formula weight	1171.38	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 7.6131(8) Å	α= 90°.
	b = 24.586(3) Å	β= 90°.
	c = 32.857(3) Å	γ = 90°.
Volume	6149.9(11) $Å^3$	
Z	4	
Density (calculated)	1.265 Mg/m^3	
Absorption coefficient	0.091 mm^{-1}	
F(000)	2520	
Crystal size	0.40 x 0.30 x 0.02 mm^3	
Theta range for data collection	2.56 to 20.81°.	
Index ranges	-6<=h<=7, -24<=k<=24, -24<=l<=32	
Reflections collected	19981	
Independent reflections	6434 [R(int) = 0.1068]	
Completeness to theta = 20.81°	99.8 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9982 and 0.8396	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6434 / 558 / 752	
Goodness-of-fit on F^2	0.980	
Final R indices [I>2sigma(I)]	R1 = 0.0641, wR2 = 0.0888	
R indices (all data)	R1 = 0.1239, wR2 = 0.1046	
Absolute structure parameter	-1.0(15)	
Largest diff. peak and hole	0.211 and -0.216 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	7648(6)	-4774(2)	5787(1)	30(1)
O(2)	11984(7)	-3669(2)	5595(1)	43(1)
O(3)	14603(6)	-5266(2)	5012(1)	32(1)
O(4)	7355(6)	-5533(2)	6535(1)	30(1)
O(5)	6247(6)	-6602(2)	6389(1)	24(1)
O(6)	3513(6)	-6357(2)	6588(1)	35(1)
C(1)	8923(9)	-5677(2)	5895(2)	18(2)
C(2)	8520(9)	-5216(2)	5586(2)	24(2)
C(3)	10186(9)	-4984(3)	5425(2)	16(2)
C(4)	10305(10)	-4468(3)	5537(2)	21(2)
C(5)	11863(10)	-4135(3)	5464(2)	30(2)
C(6)	13317(9)	-4403(2)	5230(2)	28(2)
C(7)	13335(9)	-5023(2)	5270(2)	26(2)
C(8)	11515(9)	-5284(2)	5173(2)	20(2)
C(9)	11684(9)	-5897(2)	5282(2)	28(2)
C(10)	9945(9)	-6220(2)	5279(2)	25(2)
C(11)	9001(9)	-6252(2)	5691(2)	21(2)
C(12)	7020(9)	-6416(2)	5670(2)	17(2)
C(13)	6204(9)	-6196(2)	6063(2)	18(2)
C(14)	7458(9)	-5748(2)	6204(2)	21(2)
C(15)	8705(9)	-4289(2)	5762(2)	32(2)
C(16)	11056(8)	-5222(2)	4722(2)	29(2)
C(17)	10020(8)	-6632(2)	5978(2)	27(2)
C(18)	6563(8)	-7020(2)	5598(2)	18(2)
C(19)	7268(9)	-7238(2)	5187(2)	38(2)
C(20)	4573(9)	-7094(2)	5602(2)	30(2)
C(21)	4812(11)	-6618(3)	6633(2)	27(2)
C(22)	5087(9)	-7035(3)	6966(2)	50(2)
O(1A)	11998(6)	-9427(2)	5798(1)	40(1)
O(2A)	7933(10)	-8210(2)	5786(2)	122(3)
O(3A)	5125(7)	-9432(2)	6718(1)	54(2)
O(4A)	12190(6)	-10470(2)	5285(1)	34(1)
O(5A)	13262(6)	-11423(2)	5692(1)	29(1)
O(6A)	15932(7)	-11248(2)	5429(2)	51(2)
C(1A)	10637(9)	-10314(2)	5918(2)	18(2)
C(2A)	11127(10)	-9754(2)	6103(2)	30(2)
C(3A)	9497(9)	-9436(3)	6222(2)	23(2)
C(4A)	9429(11)	-8986(3)	5999(2)	35(2)
C(5A)	7962(13)	-8597(3)	6012(2)	63(3)
C(6A)	6619(11)	-8706(2)	6333(2)	49(2)
C(7A)	6433(10)	-9316(3)	6415(2)	39(2)
C(8A)	8186(10)	-9591(2)	6537(2)	27(2)
C(9A)	7886(9)	-10207(2)	6548(2)	26(2)
C(10A)	9496(8)	-10567(2)	6630(2)	26(2)
C(11A)	10439(9)	-10772(2)	6242(2)	21(2)
C(12A)	12379(9)	-10940(2)	6316(2)	22(2)
C(13A)	13265(9)	-10904(2)	5896(2)	24(2)
C(14A)	12071(10)	-10532(2)	5653(2)	26(2)
C(15A)	10983(10)	-8942(2)	5713(2)	42(2)
C(16A)	8804(10)	-9382(2)	6954(2)	43(2)
C(17A)	9377(8)	-11235(2)	6054(2)	28(2)
C(18A)	12845(9)	-11473(2)	6535(2)	21(2)
C(19A)	11903(9)	-11554(2)	6941(2)	32(2)

C(20A)	14852(9)	-11495(2)	6604(2)	38(2)
C(21A)	14661(13)	-11526(3)	5450(2)	43(2)
C(22A)	14382(11)	-12057(3)	5226(2)	67(3)
O(1B)	11960(6)	-10242(2)	2543(1)	29(1)
O(2B)	7838(7)	-9019(2)	2445(1)	36(1)
O(3B)	4874(6)	-10279(2)	3349(1)	29(1)
O(4B)	12206(6)	-11355(2)	2081(1)	39(1)
O(5B)	13497(6)	-12220(2)	2558(1)	28(1)
O(6B)	16074(7)	-12007(2)	2250(1)	40(2)
C(1B)	10648(8)	-11123(2)	2702(2)	18(2)
C(2B)	11029(8)	-10540(2)	2853(2)	21(2)
C(3B)	9380(9)	-10235(2)	2925(2)	16(2)
C(4B)	9318(9)	-9809(2)	2682(2)	20(2)
C(5B)	7828(10)	-9428(3)	2660(2)	29(2)
C(6B)	6283(9)	-9575(2)	2932(2)	25(2)
C(7B)	6217(10)	-10176(3)	3058(2)	30(2)
C(8B)	8027(9)	-10380(2)	3230(2)	21(2)
C(9B)	7787(9)	-10995(2)	3298(2)	22(2)
C(10B)	9469(8)	-11303(2)	3417(2)	23(2)
C(11B)	10501(8)	-11541(2)	3053(2)	18(2)
C(12B)	12458(9)	-11673(2)	3145(2)	23(2)
C(13B)	13365(9)	-11673(2)	2722(2)	27(2)
C(14B)	12114(10)	-11359(2)	2450(2)	26(2)
C(15B)	10963(8)	-9753(3)	2447(2)	28(2)
C(16B)	8393(8)	-10092(2)	3636(2)	26(2)
C(17B)	9545(8)	-12045(2)	2894(2)	29(2)
C(18B)	12946(9)	-12181(2)	3404(2)	24(2)
C(19B)	11996(9)	-12209(2)	3815(2)	33(2)
C(20B)	14939(8)	-12180(2)	3484(2)	30(2)
C(21B)	14896(12)	-12323(3)	2316(2)	33(2)
C(22B)	14742(9)	-12882(3)	2139(2)	51(2)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene F.

O(1)-C(2)	1.435(6)
O(1)-C(15)	1.441(6)
O(2)-C(5)	1.227(6)
O(3)-C(7)	1.417(6)
O(4)-C(14)	1.212(6)
O(5)-C(21)	1.357(7)
O(5)-C(13)	1.463(6)
O(6)-C(21)	1.188(8)
C(1)-C(14)	1.520(8)
C(1)-C(2)	1.551(7)
C(1)-C(11)	1.566(7)
C(2)-C(3)	1.488(8)
C(3)-C(4)	1.325(7)
C(3)-C(8)	1.500(8)
C(4)-C(5)	1.461(9)
C(4)-C(15)	1.491(8)
C(5)-C(6)	1.501(8)
C(6)-C(7)	1.530(7)
C(7)-C(8)	1.560(8)
C(8)-C(16)	1.531(7)
C(8)-C(9)	1.554(7)
C(9)-C(10)	1.545(8)
C(10)-C(11)	1.534(7)
C(11)-C(17)	1.539(7)
C(11)-C(12)	1.562(8)
C(12)-C(13)	1.531(7)
C(12)-C(18)	1.545(7)
C(13)-C(14)	1.529(8)
C(18)-C(20)	1.526(8)
C(18)-C(19)	1.549(7)
C(21)-C(22)	1.512(8)
O(1A)-C(2A)	1.445(6)
O(1A)-C(15A)	1.450(7)
O(2A)-C(5A)	1.207(7)
O(3A)-C(7A)	1.435(7)
O(4A)-C(14A)	1.220(6)
O(5A)-C(21A)	1.352(8)
O(5A)-C(13A)	1.441(6)
O(6A)-C(21A)	1.186(9)
C(1A)-C(14A)	1.497(8)
C(1A)-C(2A)	1.549(7)
C(1A)-C(11A)	1.558(7)
C(2A)-C(3A)	1.518(8)
C(3A)-C(4A)	1.328(8)
C(3A)-C(8A)	1.488(8)
C(4A)-C(5A)	1.471(10)
C(4A)-C(15A)	1.515(9)
C(5A)-C(6A)	1.493(9)
C(6A)-C(7A)	1.532(8)
C(7A)-C(8A)	1.549(9)
C(8A)-C(9A)	1.532(7)
C(8A)-C(16A)	1.535(7)
C(9A)-C(10A)	1.536(8)
C(10A)-C(11A)	1.546(7)
C(11A)-C(17A)	1.528(7)
C(11A)-C(12A)	1.553(8)

C(12A)-C(18A)	1.536(7)
C(12A)-C(13A)	1.539(7)
C(13A)-C(14A)	1.517(8)
C(18A)-C(19A)	1.527(7)
C(18A)-C(20A)	1.546(8)
C(21A)-C(22A)	1.515(9)
O(1B)-C(2B)	1.442(6)
O(1B)-C(15B)	1.456(6)
O(2B)-C(5B)	1.229(6)
O(3B)-C(7B)	1.422(7)
O(4B)-C(14B)	1.213(6)
O(5B)-C(21B)	1.354(8)
O(5B)-C(13B)	1.453(6)
O(6B)-C(21B)	1.205(8)
C(1B)-C(14B)	1.506(8)
C(1B)-C(2B)	1.544(7)
C(1B)-C(11B)	1.549(7)
C(2B)-C(3B)	1.480(8)
C(3B)-C(4B)	1.319(7)
C(3B)-C(8B)	1.481(8)
C(4B)-C(5B)	1.473(8)
C(4B)-C(15B)	1.478(7)
C(5B)-C(6B)	1.520(8)
C(6B)-C(7B)	1.536(7)
C(7B)-C(8B)	1.571(8)
C(8B)-C(16B)	1.536(6)
C(8B)-C(9B)	1.542(7)
C(9B)-C(10B)	1.538(8)
C(10B)-C(11B)	1.546(7)
C(11B)-C(17B)	1.531(7)
C(11B)-C(12B)	1.554(8)
C(12B)-C(18B)	1.557(7)
C(12B)-C(13B)	1.551(8)
C(13B)-C(14B)	1.518(8)
C(18B)-C(19B)	1.533(7)
C(18B)-C(20B)	1.540(8)
C(21B)-C(22B)	1.499(8)

C(2)-O(1)-C(15)	110.0(5)
C(21)-O(5)-C(13)	115.8(5)
C(14)-C(1)-C(2)	112.1(5)
C(14)-C(1)-C(11)	102.1(5)
C(2)-C(1)-C(11)	112.8(5)
O(1)-C(2)-C(3)	105.5(5)
O(1)-C(2)-C(1)	110.1(4)
C(3)-C(2)-C(1)	110.1(5)
C(4)-C(3)-C(2)	109.0(6)
C(4)-C(3)-C(8)	125.3(7)
C(2)-C(3)-C(8)	125.7(6)
C(3)-C(4)-C(5)	123.1(7)
C(3)-C(4)-C(15)	111.4(6)
C(5)-C(4)-C(15)	125.4(6)
O(2)-C(5)-C(4)	121.7(7)
O(2)-C(5)-C(6)	122.3(7)
C(4)-C(5)-C(6)	115.9(6)
C(5)-C(6)-C(7)	113.6(5)
O(3)-C(7)-C(6)	112.0(5)
O(3)-C(7)-C(8)	108.1(5)

C(6)-C(7)-C(8)	112.6(6)
C(3)-C(8)-C(16)	109.3(5)
C(3)-C(8)-C(9)	113.9(5)
C(16)-C(8)-C(9)	109.7(5)
C(3)-C(8)-C(7)	106.6(5)
C(16)-C(8)-C(7)	111.0(5)
C(9)-C(8)-C(7)	106.2(5)
C(10)-C(9)-C(8)	115.3(5)
C(11)-C(10)-C(9)	114.9(5)
C(10)-C(11)-C(17)	109.6(5)
C(10)-C(11)-C(12)	115.3(5)
C(17)-C(11)-C(12)	110.9(5)
C(10)-C(11)-C(1)	110.5(5)
C(17)-C(11)-C(1)	107.8(5)
C(12)-C(11)-C(1)	102.4(5)
C(13)-C(12)-C(18)	112.1(5)
C(13)-C(12)-C(11)	105.4(5)
C(18)-C(12)-C(11)	118.2(5)
O(5)-C(13)-C(14)	104.8(4)
O(5)-C(13)-C(12)	111.6(5)
C(14)-C(13)-C(12)	104.8(5)
O(4)-C(14)-C(1)	126.7(6)
O(4)-C(14)-C(13)	123.1(6)
C(1)-C(14)-C(13)	109.8(5)
O(1)-C(15)-C(4)	103.9(5)
C(20)-C(18)-C(19)	108.2(5)
C(20)-C(18)-C(12)	109.6(5)
C(19)-C(18)-C(12)	112.8(5)
O(6)-C(21)-O(5)	125.5(6)
O(6)-C(21)-C(22)	124.9(7)
O(5)-C(21)-C(22)	109.6(6)
C(2A)-O(1A)-C(15A)	110.3(5)
C(21A)-O(5A)-C(13A)	116.0(6)
C(14A)-C(1A)-C(2A)	111.8(5)
C(14A)-C(1A)-C(11A)	102.1(5)
C(2A)-C(1A)-C(11A)	113.4(5)
O(1A)-C(2A)-C(3A)	105.6(5)
O(1A)-C(2A)-C(1A)	109.4(5)
C(3A)-C(2A)-C(1A)	111.2(6)
C(4A)-C(3A)-C(8A)	124.8(7)
C(4A)-C(3A)-C(2A)	108.6(7)
C(8A)-C(3A)-C(2A)	126.6(6)
C(3A)-C(4A)-C(5A)	123.8(8)
C(3A)-C(4A)-C(15A)	111.8(7)
C(5A)-C(4A)-C(15A)	124.3(6)
O(2A)-C(5A)-C(4A)	120.6(8)
O(2A)-C(5A)-C(6A)	124.3(8)
C(4A)-C(5A)-C(6A)	115.0(7)
C(5A)-C(6A)-C(7A)	111.3(6)
O(3A)-C(7A)-C(6A)	112.4(6)
O(3A)-C(7A)-C(8A)	109.4(5)
C(6A)-C(7A)-C(8A)	113.2(6)
C(3A)-C(8A)-C(9A)	111.7(5)
C(3A)-C(8A)-C(16A)	109.2(6)
C(9A)-C(8A)-C(16A)	110.8(5)
C(3A)-C(8A)-C(7A)	106.6(5)
C(9A)-C(8A)-C(7A)	108.0(6)
C(16A)-C(8A)-C(7A)	110.5(5)

C(8A)-C(9A)-C(10A)	117.1(6)
C(11A)-C(10A)-C(9A)	114.5(5)
C(17A)-C(11A)-C(10A)	109.3(5)
C(17A)-C(11A)-C(12A)	111.6(5)
C(10A)-C(11A)-C(12A)	113.5(5)
C(17A)-C(11A)-C(1A)	108.2(5)
C(10A)-C(11A)-C(1A)	111.9(5)
C(12A)-C(11A)-C(1A)	102.0(5)
C(18A)-C(12A)-C(13A)	111.6(5)
C(18A)-C(12A)-C(11A)	121.3(5)
C(13A)-C(12A)-C(11A)	105.1(5)
O(5A)-C(13A)-C(14A)	106.6(5)
O(5A)-C(13A)-C(12A)	111.6(5)
C(14A)-C(13A)-C(12A)	104.2(5)
O(4A)-C(14A)-C(1A)	125.8(6)
O(4A)-C(14A)-C(13A)	123.6(6)
C(1A)-C(14A)-C(13A)	110.2(5)
O(1A)-C(15A)-C(4A)	103.8(5)
C(19A)-C(18A)-C(12A)	114.3(5)
C(19A)-C(18A)-C(20A)	109.4(5)
C(12A)-C(18A)-C(20A)	109.1(5)
O(6A)-C(21A)-O(5A)	124.7(8)
O(6A)-C(21A)-C(22A)	125.6(8)
O(5A)-C(21A)-C(22A)	109.6(8)
C(2B)-O(1B)-C(15B)	108.4(4)
C(21B)-O(5B)-C(13B)	116.4(5)
C(14B)-C(1B)-C(2B)	113.3(5)
C(14B)-C(1B)-C(11B)	102.0(5)
C(2B)-C(1B)-C(11B)	112.9(5)
O(1B)-C(2B)-C(3B)	105.8(5)
O(1B)-C(2B)-C(1B)	109.7(4)
C(3B)-C(2B)-C(1B)	111.2(5)
C(4B)-C(3B)-C(8B)	125.1(6)
C(4B)-C(3B)-C(2B)	109.7(6)
C(8B)-C(3B)-C(2B)	125.2(6)
C(3B)-C(4B)-C(5B)	124.2(7)
C(3B)-C(4B)-C(15B)	111.1(6)
C(5B)-C(4B)-C(15B)	124.7(6)
O(2B)-C(5B)-C(4B)	122.9(7)
O(2B)-C(5B)-C(6B)	122.4(7)
C(4B)-C(5B)-C(6B)	114.7(6)
C(5B)-C(6B)-C(7B)	114.3(5)
O(3B)-C(7B)-C(6B)	112.1(5)
O(3B)-C(7B)-C(8B)	109.4(5)
C(6B)-C(7B)-C(8B)	112.0(5)
C(3B)-C(8B)-C(16B)	110.6(5)
C(3B)-C(8B)-C(9B)	114.6(5)
C(16B)-C(8B)-C(9B)	110.3(5)
C(3B)-C(8B)-C(7B)	106.9(5)
C(16B)-C(8B)-C(7B)	109.0(5)
C(9B)-C(8B)-C(7B)	105.2(5)
C(10B)-C(9B)-C(8B)	114.9(5)
C(9B)-C(10B)-C(11B)	114.4(5)
C(17B)-C(11B)-C(10B)	109.2(5)
C(17B)-C(11B)-C(1B)	108.4(5)
C(10B)-C(11B)-C(1B)	111.3(5)
C(17B)-C(11B)-C(12B)	110.7(5)
C(10B)-C(11B)-C(12B)	114.6(5)

C(1B)-C(11B)-C(12B)	102.3(5)
C(18B)-C(12B)-C(13B)	112.5(5)
C(18B)-C(12B)-C(11B)	120.1(5)
C(13B)-C(12B)-C(11B)	104.7(5)
O(5B)-C(13B)-C(14B)	107.2(5)
O(5B)-C(13B)-C(12B)	111.3(5)
C(14B)-C(13B)-C(12B)	104.4(5)
O(4B)-C(14B)-C(1B)	126.1(7)
O(4B)-C(14B)-C(13B)	123.9(6)
C(1B)-C(14B)-C(13B)	109.6(5)
O(1B)-C(15B)-C(4B)	104.6(5)
C(19B)-C(18B)-C(20B)	108.3(5)
C(19B)-C(18B)-C(12B)	113.9(5)
C(20B)-C(18B)-C(12B)	109.2(5)
O(6B)-C(21B)-O(5B)	124.8(7)
O(6B)-C(21B)-C(22B)	125.5(8)
O(5B)-C(21B)-C(22B)	109.8(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for guanacastepene F. 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)	28(3)	23(3)	38(3)	1(2)	7(3)	1(3)
O(2)	51(4)	32(3)	47(3)	-11(2)	10(3)	-10(3)
O(3)	24(3)	45(3)	26(3)	-2(2)	8(3)	-8(3)
O(4)	26(3)	44(3)	19(2)	-11(2)	5(3)	-12(3)
O(5)	25(3)	28(3)	19(2)	1(2)	0(3)	-3(3)
O(6)	17(4)	56(4)	32(3)	10(3)	9(3)	8(3)
C(1)	15(5)	22(4)	16(3)	0(3)	-8(4)	-4(4)
C(2)	30(5)	20(4)	22(4)	-2(3)	-4(4)	1(4)
C(3)	16(5)	20(4)	12(4)	9(3)	0(4)	-3(4)
C(4)	29(5)	16(4)	18(4)	2(3)	-2(4)	3(4)
C(5)	36(6)	30(5)	24(4)	5(4)	-4(4)	-9(5)
C(6)	15(5)	40(5)	29(4)	3(4)	-3(4)	-10(4)
C(7)	32(6)	36(5)	11(4)	-6(3)	8(4)	5(4)
C(8)	25(5)	28(4)	7(3)	0(3)	-5(4)	-6(4)
C(9)	26(5)	28(4)	28(4)	3(3)	0(4)	5(4)
C(10)	33(5)	21(4)	22(4)	-3(3)	4(4)	-4(4)
C(11)	17(5)	22(4)	24(4)	0(3)	-2(4)	3(4)
C(12)	17(5)	18(4)	17(3)	-5(3)	-5(4)	-6(4)
C(13)	19(5)	19(4)	17(4)	3(3)	4(4)	-2(4)
C(14)	22(5)	25(4)	14(4)	3(3)	-8(4)	4(4)
C(15)	37(6)	20(4)	40(4)	-8(4)	2(4)	5(4)
C(16)	27(5)	36(4)	24(4)	4(3)	5(4)	-3(4)
C(17)	14(5)	41(5)	26(4)	4(3)	1(4)	5(4)
C(18)	12(5)	26(4)	17(4)	0(3)	-9(4)	-6(4)
C(19)	46(6)	29(4)	38(4)	-9(3)	6(4)	-9(4)
C(20)	30(5)	26(4)	34(4)	-13(3)	-6(4)	-3(4)
C(21)	24(6)	32(5)	26(5)	0(4)	3(5)	-10(5)
C(22)	34(6)	80(6)	37(4)	34(4)	10(4)	-4(5)
O(1A)	44(4)	31(3)	43(3)	15(3)	11(3)	-6(3)
O(2A)	158(7)	72(4)	135(5)	78(4)	80(5)	75(5)
O(3A)	58(4)	53(4)	52(3)	9(3)	18(3)	33(3)
O(4A)	32(3)	49(3)	21(2)	1(2)	-1(3)	11(3)
O(5A)	26(4)	23(3)	38(3)	-3(2)	7(3)	4(3)
O(6A)	29(4)	75(4)	49(3)	-6(3)	9(3)	5(3)
C(1A)	15(5)	28(4)	10(3)	4(3)	3(3)	-2(4)
C(2A)	42(6)	22(4)	25(4)	-2(4)	-4(4)	-11(4)
C(3A)	27(5)	18(4)	25(4)	-5(4)	-10(4)	-2(4)
C(4A)	49(6)	27(5)	28(4)	3(4)	-5(5)	12(5)
C(5A)	89(8)	52(6)	46(5)	19(4)	28(6)	31(6)
C(6A)	72(7)	37(5)	39(4)	-4(4)	21(5)	29(5)
C(7A)	59(7)	38(5)	20(4)	9(4)	3(5)	23(5)
C(8A)	38(6)	18(4)	26(4)	3(3)	9(4)	6(4)
C(9A)	22(5)	39(4)	19(4)	6(3)	11(4)	6(4)
C(10A)	32(5)	18(4)	27(4)	12(3)	5(4)	6(4)
C(11A)	23(5)	27(4)	12(4)	-2(3)	-1(4)	-2(4)
C(12A)	19(5)	23(4)	24(4)	0(3)	3(4)	-6(4)
C(13A)	23(5)	25(4)	23(4)	4(3)	3(4)	10(4)
C(14A)	21(5)	32(4)	24(4)	-1(4)	-8(4)	-7(4)
C(15A)	59(7)	11(4)	56(5)	17(4)	8(5)	-2(4)
C(16A)	65(7)	47(5)	16(4)	-5(4)	-5(4)	9(5)
C(17A)	18(5)	39(5)	27(4)	2(4)	3(4)	-7(4)
C(18A)	25(5)	19(4)	19(4)	4(3)	-6(4)	1(4)
C(19A)	45(6)	24(4)	27(4)	6(3)	-1(4)	1(4)

C(20A)	36(6)	29(5)	48(5)	6(4)	-11(5)	4(4)
C(21A)	45(7)	56(6)	29(5)	-9(5)	2(6)	25(6)
C(22A)	77(8)	68(6)	56(5)	-31(5)	13(5)	12(6)
O(1B)	25(3)	31(3)	32(3)	13(2)	10(3)	-1(3)
O(2B)	49(4)	27(3)	31(3)	13(2)	8(3)	9(3)
O(3B)	22(3)	32(3)	31(3)	1(2)	2(3)	6(3)
O(4B)	39(4)	57(3)	21(2)	-1(2)	0(3)	17(3)
O(5B)	19(3)	31(3)	34(3)	-10(2)	6(3)	-1(3)
O(6B)	29(4)	53(4)	38(3)	-2(3)	9(3)	1(3)
C(1B)	10(5)	25(4)	19(4)	-5(3)	-6(4)	-3(4)
C(2B)	21(5)	16(4)	25(4)	1(3)	3(4)	-3(4)
C(4B)	21(5)	25(4)	13(4)	2(3)	9(4)	5(4)
C(5B)	42(6)	34(5)	12(4)	-13(4)	0(4)	7(5)
C(6B)	20(5)	31(4)	23(4)	-6(3)	-4(4)	9(4)
C(7B)	33(6)	28(5)	29(4)	0(4)	6(4)	-2(4)
C(8B)	24(5)	14(4)	24(4)	1(3)	-6(4)	2(4)
C(9B)	12(5)	24(4)	29(4)	-6(3)	0(4)	-2(4)
C(10B)	23(5)	19(4)	26(4)	6(3)	6(4)	-8(4)
C(11B)	9(5)	15(4)	29(4)	0(3)	4(4)	-5(4)
C(12B)	17(5)	25(4)	27(4)	-2(3)	-4(4)	4(4)
C(13B)	28(5)	14(4)	38(4)	-7(3)	-2(4)	4(4)
C(14B)	30(5)	21(4)	28(4)	1(4)	-6(5)	-2(4)
C(15B)	26(5)	30(4)	28(4)	7(4)	-6(4)	-7(4)
C(16B)	21(5)	33(4)	23(4)	-9(3)	-9(4)	3(4)
C(17B)	20(5)	26(4)	41(4)	-4(4)	-11(4)	-5(4)
C(18B)	20(5)	18(4)	33(4)	-5(3)	-2(4)	-1(4)
C(19B)	36(5)	29(4)	34(4)	2(3)	0(4)	-8(4)
C(20B)	22(5)	27(4)	40(4)	-1(4)	4(4)	5(4)
C(21B)	41(7)	42(6)	17(4)	0(4)	-11(5)	6(5)
C(22B)	33(6)	75(6)	44(4)	-33(5)	4(5)	10(5)

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

	x	y	z	U(eq)
H(3A)	15331	-5029	4937	47
H(1A)	10055	-5600	6038	21
H(2A)	7779	-5357	5358	29
H(6A)	14456	-4258	5326	34
H(6B)	13197	-4306	4938	34
H(7A)	13646	-5115	5558	32
H(9A)	12504	-6068	5087	33
H(9B)	12214	-5927	5556	33
H(10A)	9141	-6051	5079	30
H(10B)	10193	-6595	5185	30
H(12A)	6489	-6205	5440	21
H(13A)	4990	-6054	6017	22
H(15A)	9012	-4153	6037	39
H(15B)	8081	-3998	5612	39
H(16A)	10930	-4835	4656	43
H(16B)	9950	-5411	4665	43
H(16C)	11995	-5380	4556	43
H(17A)	11258	-6524	5985	40
H(17B)	9929	-7008	5879	40
H(17C)	9523	-6609	6252	40
H(18A)	7081	-7242	5823	22
H(19A)	8548	-7196	5178	56
H(19B)	6740	-7031	4963	56
H(19C)	6963	-7623	5159	56
H(20A)	4100	-6962	5861	45
H(20B)	4288	-7480	5570	45
H(20C)	4052	-6886	5378	45
H(22A)	4049	-7046	7141	75
H(22B)	6119	-6935	7128	75
H(22C)	5273	-7393	6843	75
H(3AA)	4591	-9144	6778	82
H(1AA)	9527	-10281	5757	21
H(2AA)	11909	-9804	6344	36
H(6AA)	5472	-8557	6245	59
H(6AB)	6964	-8518	6587	59
H(7AA)	6036	-9490	6156	47
H(9AA)	7374	-10317	6284	32
H(9AB)	6999	-10285	6761	32
H(10C)	10346	-10359	6796	31
H(10D)	9120	-10886	6792	31
H(12B)	12908	-10642	6484	26
H(13B)	14479	-10752	5917	28
H(15C)	10592	-8935	5426	50
H(15D)	11677	-8610	5770	50
H(16D)	9905	-9563	7029	64
H(16E)	7907	-9462	7159	64
H(16F)	8995	-8989	6940	64
H(17D)	8166	-11114	6009	42
H(17E)	9379	-11548	6238	42
H(17F)	9904	-11340	5793	42
H(18B)	12516	-11781	6353	25
H(19D)	12263	-11901	7061	48

H(19E)	10630	-11555	6896	48
H(19F)	12211	-11256	7127	48
H(20D)	15161	-11837	6739	56
H(20E)	15212	-11189	6776	56
H(20F)	15457	-11472	6341	56
H(22D)	15396	-12130	5051	100
H(22E)	13318	-12033	5060	100
H(22F)	14253	-12353	5424	100
H(3BA)	4190	-10011	3359	43
H(1BA)	9536	-11125	2540	21
H(2BA)	11742	-10553	3109	25
H(6BA)	5181	-9483	2787	30
H(6BB)	6335	-9348	3181	30
H(7BA)	5945	-10395	2809	36
H(9BA)	6901	-11050	3515	26
H(9BB)	7313	-11158	3046	26
H(10E)	9149	-11604	3603	27
H(10F)	10248	-11052	3569	27
H(12C)	12935	-11351	3295	28
H(13C)	14542	-11493	2735	32
H(15E)	10716	-9732	2152	34
H(15F)	11615	-9423	2531	34
H(16G)	8545	-9701	3588	38
H(16H)	9465	-10241	3758	38
H(16I)	7402	-10150	3822	38
H(17G)	10174	-12190	2657	44
H(17H)	8346	-11946	2814	44
H(17I)	9500	-12322	3108	44
H(18C)	12645	-12514	3244	28
H(19G)	12349	-12541	3958	49
H(19H)	10724	-12215	3769	49
H(19I)	12308	-11891	3979	49
H(20G)	15256	-12504	3642	45
H(20H)	15257	-11854	3639	45
H(20I)	15570	-12183	3225	45
H(22G)	15751	-12954	1961	76
H(22H)	13655	-12909	1980	76
H(22I)	14718	-13151	2359	76

Table 1. Crystal data and structure refinement for guanacastepene G.

Identification code	shana	
Empirical formula	C22 H30 O5	
Formula weight	374.46	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.9147(11) Å	α= 90°.
	b = 10.2697(13) Å	β= 90°.
	c = 21.833(3) Å	γ = 90°.
Volume	1998.9(4) $Å^3$	
Z	4	
Density (calculated)	1.244 Mg/m^3	
Absorption coefficient	0.087 mm^{-1}	
F(000)	808	
Crystal size	0.10 x 0.08 x 0.05 mm^3	
Theta range for data collection	1.87 to 25.75°.	
Index ranges	-10<=h<=10, -12<=k<=11, -26<=l<=26	
Reflections collected	10687	
Independent reflections	3760 [R(int) = 0.0881]	
Absorption correction	SADABS	
Max. and min. transmission	1 and 0.586613	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2434 / 0 / 244	
Goodness-of-fit on F^2	1.086	
Final R indices [I>2sigma(I)]	R1 = 0.0502, wR2 = 0.1065	
R indices (all data)	R1 = 0.1327, wR2 = 0.1485	
Absolute structure parameter	0.16(201)	
Largest diff. peak and hole	0.220 and -0.209 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	9752(3)	8575(2)	1449(1)	31(1)
O(2)	12438(5)	8813(3)	-187(1)	68(1)
O(3)	8432(3)	9556(2)	3618(1)	27(1)
O(4)	6417(4)	8248(3)	3651(2)	51(1)
O(5)	8145(3)	10319(3)	2393(1)	36(1)
C(1)	10247(6)	8471(4)	830(2)	38(1)
C(2)	11883(6)	8759(4)	865(2)	32(1)
C(3)	12880(7)	8935(4)	341(2)	47(2)
C(4)	14496(6)	9224(5)	490(2)	54(2)
C(5)	14753(5)	9775(4)	1140(2)	43(1)
C(6)	13954(5)	8999(4)	1641(2)	28(1)
C(7)	14079(5)	9748(4)	2250(2)	32(1)
C(8)	13340(5)	9090(4)	2804(2)	30(1)
C(9)	11702(4)	9506(4)	2930(2)	18(1)
C(10)	10758(5)	8459(4)	3287(2)	21(1)
C(11)	9112(4)	8784(4)	3138(2)	22(1)
C(12)	9179(5)	9663(4)	2571(2)	25(1)
C(14)	11013(5)	8580(4)	1857(2)	24(1)
C(14)	10776(4)	9667(4)	2333(2)	19(1)
C(15)	12357(5)	8808(4)	1448(2)	24(1)
C(16)	14711(5)	7648(4)	1720(2)	47(1)
C(17)	11662(5)	10813(4)	3270(2)	27(1)
C(18)	11032(5)	8240(4)	3978(2)	27(1)
C(19)	10061(5)	7109(4)	4202(2)	40(1)
C(20)	12671(5)	7975(5)	4146(2)	47(1)
C(21)	7093(5)	9162(4)	3848(2)	34(1)
C(22)	6630(5)	9992(4)	4370(2)	47(1)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene G.

O(1)-C(1)	1.426(4)
O(1)-C(14)	1.434(5)
O(2)-C(3)	1.223(5)
O(3)-C(21)	1.356(5)
O(3)-C(11)	1.447(4)
O(4)-C(21)	1.195(5)
O(5)-C(12)	1.207(5)
C(1)-C(2)	1.491(6)
C(2)-C(15)	1.342(5)
C(2)-C(3)	1.460(6)
C(3)-C(4)	1.507(7)
C(4)-C(5)	1.544(6)
C(5)-C(6)	1.530(5)
C(6)-C(15)	1.498(6)
C(6)-C(7)	1.541(5)
C(6)-C(16)	1.553(6)
C(7)-C(8)	1.533(5)
C(8)-C(9)	1.546(6)
C(9)-C(17)	1.535(5)
C(9)-C(14)	1.552(5)
C(9)-C(10)	1.572(5)
C(10)-C(11)	1.540(5)
C(10)-C(18)	1.545(5)
C(11)-C(12)	1.532(5)
C(12)-C(14)	1.516(5)
C(14)-C(15)	1.512(5)
C(14)-C(14)	1.539(5)
C(18)-C(19)	1.529(6)
C(18)-C(20)	1.531(6)
C(21)-C(22)	1.483(6)
C(1)-O(1)-C(14)	110.3(3)
C(21)-O(3)-C(11)	118.2(3)
O(1)-C(1)-C(2)	103.8(3)
C(15)-C(2)-C(3)	123.2(5)
C(15)-C(2)-C(1)	111.4(4)
C(3)-C(2)-C(1)	125.4(4)
O(2)-C(3)-C(2)	122.0(5)
O(2)-C(3)-C(4)	122.1(5)
C(2)-C(3)-C(4)	115.9(4)
C(3)-C(4)-C(5)	114.4(4)
C(6)-C(5)-C(4)	113.4(4)
C(15)-C(6)-C(5)	108.0(3)
C(15)-C(6)-C(7)	112.1(3)
C(5)-C(6)-C(7)	108.9(3)
C(15)-C(6)-C(16)	109.1(3)
C(5)-C(6)-C(16)	110.1(3)
C(7)-C(6)-C(16)	108.6(3)
C(8)-C(7)-C(6)	115.4(4)
C(7)-C(8)-C(9)	115.1(3)
C(17)-C(9)-C(8)	110.5(3)
C(17)-C(9)-C(14)	107.5(3)
C(8)-C(9)-C(14)	112.5(3)
C(17)-C(9)-C(10)	110.2(3)
C(8)-C(9)-C(10)	113.9(3)
C(14)-C(9)-C(10)	101.8(3)

C(11)-C(10)-C(18)	112.9(3)
C(11)-C(10)-C(9)	104.9(3)
C(18)-C(10)-C(9)	120.0(3)
O(3)-C(11)-C(12)	106.2(3)
O(3)-C(11)-C(10)	111.4(3)
C(12)-C(11)-C(10)	105.1(3)
O(5)-C(12)-C(14)	127.2(4)
O(5)-C(12)-C(11)	124.0(4)
C(14)-C(12)-C(11)	108.4(3)
O(1)-C(14)-C(15)	104.8(3)
O(1)-C(14)-C(14)	108.3(3)
C(15)-C(14)-C(14)	113.2(3)
C(12)-C(14)-C(14)	111.0(3)
C(12)-C(14)-C(9)	102.1(3)
C(14)-C(14)-C(9)	114.6(3)
C(2)-C(15)-C(6)	124.8(4)
C(2)-C(15)-C(14)	107.7(4)
C(6)-C(15)-C(14)	127.4(3)
C(19)-C(18)-C(20)	109.2(4)
C(19)-C(18)-C(10)	109.5(3)
C(20)-C(18)-C(10)	114.2(3)
O(4)-C(21)-O(3)	123.1(4)
O(4)-C(21)-C(22)	125.9(4)
O(3)-C(21)-C(22)	111.0(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for guanacastepene G. 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)	43(2)	30(2)	21(2)	2(1)	-11(2)	-6(2)
O(2)	116(3)	69(2)	19(2)	4(2)	9(2)	9(3)
O(3)	25(2)	24(2)	32(2)	-2(1)	7(1)	-2(1)
O(4)	30(2)	51(2)	72(3)	2(2)	7(2)	-11(2)
O(5)	30(2)	39(2)	41(2)	8(2)	-4(2)	6(2)
C(1)	73(4)	27(3)	16(2)	-2(2)	-8(2)	-7(3)
C(2)	60(4)	14(2)	22(3)	1(2)	2(3)	5(2)
C(3)	85(5)	28(3)	28(3)	2(2)	11(3)	8(3)
C(4)	74(4)	54(3)	35(3)	9(2)	22(3)	4(3)
C(5)	50(3)	46(3)	34(3)	4(2)	17(2)	6(3)
C(6)	31(3)	26(3)	29(2)	-1(2)	7(2)	6(2)
C(7)	22(3)	37(3)	37(3)	0(2)	5(2)	-3(2)
C(8)	26(3)	38(3)	25(3)	-1(2)	-4(2)	3(2)
C(9)	22(2)	16(2)	17(2)	-1(2)	-2(2)	2(2)
C(10)	28(3)	18(2)	17(2)	-5(2)	-2(2)	5(2)
C(11)	26(3)	22(2)	18(2)	3(2)	2(2)	-2(2)
C(12)	25(3)	20(2)	29(3)	-3(2)	-4(2)	-7(2)
C(14)	40(3)	13(2)	20(2)	2(2)	-6(2)	0(2)
C(14)	23(2)	13(2)	22(2)	0(2)	0(2)	-3(2)
C(15)	41(3)	6(2)	23(3)	-1(2)	2(2)	4(2)
C(16)	51(3)	40(3)	49(3)	-3(2)	4(3)	21(3)
C(17)	30(3)	25(2)	25(2)	-2(2)	-3(2)	-7(2)
C(18)	34(3)	24(3)	22(2)	1(2)	-1(2)	3(2)
C(19)	42(3)	40(3)	38(3)	14(2)	7(2)	7(3)
C(20)	43(3)	69(4)	30(3)	16(2)	-9(2)	6(3)
C(21)	31(3)	30(3)	42(3)	16(2)	4(2)	-1(2)
C(22)	42(3)	49(3)	49(3)	4(2)	15(3)	9(3)

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

	x	y	z	U(eq)
H(1A)	9725(6)	9110(4)	565(2)	46
H(1B)	10068(6)	7584(4)	667(2)	46
H(4A)	14885(6)	9857(5)	187(2)	65
H(4B)	15085(6)	8412(5)	446(2)	65
H(5A)	15843(5)	9782(4)	1226(2)	52
H(5B)	14396(5)	10687(4)	1152(2)	52
H(7A)	15154(5)	9882(4)	2343(2)	38
H(7B)	13619(5)	10618(4)	2195(2)	38
H(8A)	13948(5)	9281(4)	3172(2)	35
H(8B)	13361(5)	8135(4)	2740(2)	35
H(10A)	10971(5)	7607(4)	3083(2)	25
H(11A)	8518(4)	7977(4)	3055(2)	26
H(14A)	11102(5)	7718(4)	2067(2)	29
H(14B)	11003(4)	10531(4)	2142(2)	23
H(16A)	15757(5)	7766(4)	1846(2)	70
H(16B)	14679(5)	7175(4)	1330(2)	70
H(16C)	14174(5)	7148(4)	2034(2)	70
H(17A)	10618(5)	11063(4)	3347(2)	40
H(17B)	12150(5)	11482(4)	3020(2)	40
H(17C)	12192(5)	10728(4)	3661(2)	40
H(18A)	10707(5)	9043(4)	4200(2)	32
H(19A)	9010(5)	7274(4)	4095(2)	60
H(19B)	10156(5)	7028(4)	4648(2)	60
H(19C)	10394(5)	6300(4)	4007(2)	60
H(20A)	13297(5)	8699(5)	4003(2)	71
H(20B)	13002(5)	7166(5)	3950(2)	71
H(20C)	12763(5)	7891(5)	4591(2)	71
H(22A)	7381(5)	10676(4)	4435(2)	70
H(22B)	6547(5)	9458(4)	4740(2)	70
H(22C)	5657(5)	10392(4)	4280(2)	70

Table 1. Crystal data and structure refinement for guanacastepene H.

Identification code	cr115b	
Empirical formula	C22 H29 N O5	
Formula weight	387.46	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 8.0197(16) Å	α= 90°.
	b = 15.304(3) Å	β= 109.79(3)°.
	c = 8.2962(17) Å	γ = 90°.
Volume	958.1(3) $Å^3$	
Z	2	
Density (calculated)	1.343 Mg/m^3	
Absorption coefficient	0.095 mm^{-1}	
F(000)	416	
Crystal size	0.2 x 0.15 x 0.1 mm^3	
Theta range for data collection	2.61 to 20.82°.	
Index ranges	-8<=h<=7, -15<=k<=15, -6<=l<=8	
Reflections collected	3352	
Independent reflections	1879 [R(int) = 0.0584]	
Completeness to theta = 20.82°	99.7 %	
Absorption correction	SADABS	
Max. and min. transmission	1 and 0.614698	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1879 / 1 / 337	
Goodness-of-fit on F^2	1.095	
Final R indices [I>2sigma(I)]	R1 = 0.0611, wR2 = 0.1138	
R indices (all data)	R1 = 0.0779, wR2 = 0.1219	
Absolute structure parameter	0(2)	
Largest diff. peak and hole	0.167 and -0.177 $e.Å^{-3}$	

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

	x	y	z	U(eq)
N(1)	1760(6)	4630(3)	3618(6)	29(1)
O(1)	299(7)	6471(3)	6773(8)	90(2)
O(2)	592(5)	4573(3)	5795(5)	45(1)
O(3)	2466(5)	3485(3)	857(6)	48(1)
O(4)	1150(5)	4723(3)	-701(5)	47(1)
O(5)	5438(5)	3651(3)	362(6)	47(1)
C(1)	3448(7)	5044(3)	1775(7)	26(2)
C(2)	2729(7)	5235(4)	3005(7)	26(2)
C(3)	2700(8)	6057(4)	3906(7)	30(2)
C(4)	1772(8)	5906(4)	4996(8)	36(2)
C(5)	1272(8)	6605(5)	5975(9)	48(2)
C(6)	1990(10)	7494(5)	5838(11)	52(2)
C(7)	3490(9)	7513(5)	5148(10)	45(2)
C(8)	3204(8)	6963(4)	3520(8)	34(2)
C(9)	4904(9)	6983(4)	3073(9)	41(2)
C(10)	4846(11)	6524(5)	1430(9)	43(2)
C(11)	4991(7)	5531(4)	1468(7)	28(2)
C(12)	4966(8)	5170(4)	-322(8)	29(2)
C(13)	4114(8)	4265(4)	-491(9)	33(2)
C(14)	2746(8)	4333(4)	403(8)	30(2)
C(15)	1275(7)	4977(4)	4897(8)	29(2)
C(16)	1607(9)	7325(5)	2018(11)	58(2)
C(17)	6708(9)	5247(5)	2905(9)	43(2)
C(18)	6681(8)	5178(4)	-754(8)	36(2)
C(19)	7564(9)	6065(5)	-698(10)	66(2)
C(20)	6338(8)	4773(5)	-2540(8)	48(2)
C(21)	1140(9)	3351(5)	1645(9)	45(2)
C(22)	1849(9)	3672(4)	3473(9)	40(2)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene H.

N(1)-C(15)	1.356(7)
N(1)-C(2)	1.410(7)
N(1)-C(22)	1.475(8)
O(1)-C(5)	1.199(7)
O(2)-C(15)	1.231(7)
O(3)-C(14)	1.391(7)
O(3)-C(21)	1.440(7)
O(4)-C(14)	1.429(7)
O(5)-C(13)	1.415(7)
C(1)-C(2)	1.363(7)
C(1)-C(14)	1.537(8)
C(1)-C(11)	1.538(8)
C(2)-C(3)	1.468(8)
C(3)-C(4)	1.371(8)
C(3)-C(8)	1.508(8)
C(4)-C(5)	1.478(9)
C(4)-C(15)	1.471(9)
C(5)-C(6)	1.497(10)
C(6)-C(7)	1.497(10)
C(7)-C(8)	1.542(9)
C(8)-C(9)	1.530(9)
C(8)-C(16)	1.556(9)
C(9)-C(10)	1.520(9)
C(10)-C(11)	1.523(8)
C(11)-C(17)	1.547(9)
C(11)-C(12)	1.578(8)
C(12)-C(13)	1.530(8)
C(12)-C(18)	1.535(8)
C(13)-C(14)	1.522(8)
C(18)-C(19)	1.524(9)
C(18)-C(20)	1.542(8)
C(21)-C(22)	1.510(10)
C(15)-N(1)-C(2)	111.4(5)
C(15)-N(1)-C(22)	119.2(5)
C(2)-N(1)-C(22)	125.2(5)
C(14)-O(3)-C(21)	117.9(5)
C(2)-C(1)-C(14)	124.4(4)
C(2)-C(1)-C(11)	126.0(5)
C(14)-C(1)-C(11)	109.5(5)
C(1)-C(2)-N(1)	123.6(5)
C(1)-C(2)-C(3)	130.5(5)
N(1)-C(2)-C(3)	105.9(5)
C(4)-C(3)-C(2)	107.3(5)
C(4)-C(3)-C(8)	122.6(5)
C(2)-C(3)-C(8)	128.9(5)
C(3)-C(4)-C(5)	123.3(6)
C(3)-C(4)-C(15)	108.9(5)
C(5)-C(4)-C(15)	127.7(6)
O(1)-C(5)-C(4)	121.8(7)
O(1)-C(5)-C(6)	122.4(6)
C(4)-C(5)-C(6)	115.7(6)
C(5)-C(6)-C(7)	115.2(6)
C(6)-C(7)-C(8)	115.1(6)
C(3)-C(8)-C(9)	113.3(5)
C(3)-C(8)-C(7)	106.7(5)

C(9)-C(8)-C(7)	108.7(5)
C(3)-C(8)-C(16)	106.9(5)
C(9)-C(8)-C(16)	111.0(6)
C(7)-C(8)-C(16)	110.2(6)
C(10)-C(9)-C(8)	116.7(6)
C(9)-C(10)-C(11)	117.6(6)
C(10)-C(11)-C(1)	115.3(5)
C(10)-C(11)-C(17)	109.7(5)
C(1)-C(11)-C(17)	107.0(5)
C(10)-C(11)-C(12)	110.7(5)
C(1)-C(11)-C(12)	103.4(5)
C(17)-C(11)-C(12)	110.6(5)
C(13)-C(12)-C(18)	113.2(5)
C(13)-C(12)-C(11)	105.5(5)
C(18)-C(12)-C(11)	119.4(5)
O(5)-C(13)-C(14)	110.1(5)
O(5)-C(13)-C(12)	108.6(5)
C(14)-C(13)-C(12)	105.5(5)
O(3)-C(14)-O(4)	111.9(5)
O(3)-C(14)-C(13)	106.1(5)
O(4)-C(14)-C(13)	110.7(5)
O(3)-C(14)-C(1)	120.8(5)
O(4)-C(14)-C(1)	101.7(4)
C(13)-C(14)-C(1)	105.4(5)
O(2)-C(15)-N(1)	125.5(6)
O(2)-C(15)-C(4)	128.3(6)
N(1)-C(15)-C(4)	106.2(5)
C(19)-C(18)-C(12)	116.4(5)
C(19)-C(18)-C(20)	108.5(6)
C(12)-C(18)-C(20)	109.8(5)
O(3)-C(21)-C(22)	108.9(5)
N(1)-C(22)-C(21)	113.1(6)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	39(3)	31(3)	20(3)	-6(3)	15(3)	-2(2)
O(1)	131(5)	62(4)	119(5)	-11(3)	97(4)	-2(3)
O(2)	48(3)	55(3)	38(3)	5(2)	23(2)	-6(2)
O(3)	60(3)	35(3)	61(3)	-14(2)	36(3)	-13(2)
O(4)	40(3)	72(3)	29(2)	-6(2)	14(2)	6(2)
O(5)	53(3)	29(2)	62(3)	0(2)	22(2)	8(2)
C(1)	38(4)	15(3)	23(4)	4(3)	8(3)	-2(3)
C(2)	36(3)	23(4)	20(4)	2(3)	13(3)	-2(3)
C(3)	35(3)	33(4)	19(4)	0(3)	5(3)	-5(3)
C(4)	35(4)	42(5)	33(4)	-5(4)	14(3)	5(3)
C(5)	45(4)	64(5)	46(5)	-11(4)	28(4)	-1(4)
C(6)	60(5)	52(5)	57(5)	-26(5)	37(5)	1(5)
C(7)	42(4)	41(5)	49(5)	-5(4)	9(4)	2(4)
C(8)	37(4)	28(4)	39(4)	1(3)	13(3)	4(3)
C(9)	49(4)	31(4)	51(5)	-7(4)	29(4)	-13(4)
C(10)	63(5)	38(5)	41(5)	10(4)	33(4)	5(4)
C(11)	34(4)	24(4)	26(4)	0(3)	11(3)	2(3)
C(12)	28(3)	34(4)	21(4)	10(3)	2(3)	14(3)
C(13)	35(4)	25(4)	37(4)	-1(3)	11(3)	1(3)
C(14)	33(4)	24(4)	37(4)	8(3)	19(3)	8(3)
C(15)	27(3)	41(4)	18(4)	-4(3)	5(3)	-8(3)
C(16)	47(5)	54(5)	66(6)	19(5)	10(5)	0(4)
C(17)	55(5)	49(5)	26(4)	3(4)	15(4)	5(4)
C(18)	36(4)	41(4)	33(4)	5(4)	14(3)	5(4)
C(19)	69(5)	70(5)	80(6)	-13(5)	53(5)	-22(4)
C(20)	52(4)	65(5)	38(4)	4(4)	29(4)	9(4)
C(21)	52(5)	44(5)	46(5)	-10(4)	26(4)	-18(4)
C(22)	36(4)	37(5)	59(6)	9(4)	30(4)	-9(3)

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

	x	y	z	U(eq)
H(4A)	1079	4651	-1726	70
H(5A)	4984	3151	284	71
H(19A)	6792	6441	-1600	99
H(19B)	8700	5987	-881	99
H(19C)	7767	6337	421	99
H(20A)	5619	5175	-3422	72
H(20B)	5705	4219	-2620	72
H(20C)	7471	4669	-2713	72
H(12)	4050(50)	5490(30)	-1200(60)	0(11)
H(17C)	6710(70)	4560(40)	2740(70)	49(19)
H(17B)	6680(70)	5320(40)	4010(80)	34(17)
H(6A)	2200(60)	7810(30)	7000(70)	19(14)
H(13A)	3410(90)	4100(40)	-1800(90)	70(20)
H(7A)	4010(70)	8030(40)	5030(80)	50(20)
H(17A)	7890(110)	5540(60)	2630(110)	120(30)
H(16C)	2040(80)	7860(40)	1600(80)	50(20)
H(18)	7490(60)	4730(30)	160(70)	30(16)
H(7A)	4490(60)	7330(30)	6040(70)	12(15)
H(16B)	1100(110)	6840(60)	880(120)	130(40)
H(16A)	430(100)	7460(60)	2410(110)	110(30)
H(9B)	5060(70)	7610(50)	2790(80)	50(20)
H(10B)	5890(100)	6730(50)	980(100)	90(30)
H(22B)	1010(60)	3450(30)	3900(60)	18(14)
H(22A)	3260(80)	3500(40)	4120(70)	47(16)
H(10A)	3850(70)	6710(30)	590(70)	22(17)
H(9A)	5950(120)	6630(60)	4150(130)	150(40)
H(21B)	-210(90)	3660(50)	930(80)	80(20)
H(21A)	1040(70)	2550(50)	1720(80)	64(19)
H(6B)	1070(60)	7880(30)	5130(70)	28(18)

Table 1. Crystal data and structure refinement for guanacastepene I.

Identification code	cr115-8	
Empirical formula	C21 H30 O5	
Formula weight	362.45	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 10.186(2) Å	α= 90°.
	b = 6.4521(13) Å	β= 94.92(3)°.
	c = 13.958(3) Å	γ = 90°.
Volume	913.9(3) $Å^3$	
Z	2	
Density (calculated)	1.317 Mg/m^3	
Absorption coefficient	0.093 mm^{-1}	
F(000)	392	
Crystal size	0.3 x 0.1 x 0.05 mm^3	
Theta range for data collection	2.01 to 20.79°.	
Index ranges	-9<=h<=10, -5<=k<=6, -13<=l<=13	
Reflections collected	3176	
Independent reflections	1688 [R(int) = 0.0616]	
Completeness to theta = 20.79°	99.8 %	
Absorption correction	SADABS	
Max. and min. transmission	1 and 0.642329	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1688 / 1 / 235	
Goodness-of-fit on F^2	0.952	
Final R indices [I>2sigma(I)]	R1 = 0.0548, wR2 = 0.1161	
R indices (all data)	R1 = 0.0747, wR2 = 0.1289	
Absolute structure parameter	5(3)	
Largest diff. peak and hole	0.206 and -0.241 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	5703(4)	7987(7)	10884(3)	25(1)
O(2)	8533(4)	9229(7)	9203(2)	24(1)
O(3)	12653(3)	8430(7)	11015(3)	24(1)
O(4)	9919(3)	8486(7)	10574(2)	16(1)
O(5)	13415(4)	6971(7)	13103(2)	21(1)
C(1)	11004(5)	9480(9)	12078(4)	15(2)
C(2)	9908(6)	9466(9)	11454(4)	15(2)
C(3)	8574(5)	10279(9)	11526(4)	11(2)
C(4)	7786(6)	9510(9)	10791(4)	15(2)
C(5)	6329(5)	9871(10)	10613(4)	19(2)
C(6)	5919(5)	11737(11)	11205(4)	21(2)
C(7)	6636(5)	11736(12)	12222(4)	21(2)
C(8)	8136(5)	11877(11)	12212(4)	16(2)
C(9)	8743(5)	11699(12)	13250(4)	23(2)
C(10)	10250(5)	11904(12)	13396(4)	23(2)
C(11)	11052(5)	9958(10)	13158(4)	14(2)
C(12)	12560(5)	10378(10)	13412(4)	17(2)
C(13)	13252(6)	9019(10)	12708(4)	16(2)
C(14)	12303(6)	8890(9)	11811(4)	16(2)
C(15)	8581(5)	8353(11)	10112(4)	18(2)
C(16)	8485(6)	14037(10)	11803(4)	25(2)
C(17)	10579(5)	8037(10)	13686(4)	20(2)
C(18)	13168(5)	10141(10)	14459(4)	16(2)
C(19)	12558(6)	11542(12)	15183(4)	30(2)
C(20)	14654(5)	10537(11)	14488(4)	23(2)
C(21)	14235(6)	5672(11)	12575(4)	31(2)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene I.

O(1)-C(5)	1.438(7)
O(2)-C(15)	1.386(6)
O(3)-C(14)	1.232(6)
O(4)-C(2)	1.383(6)
O(4)-C(15)	1.460(6)
O(5)-C(21)	1.431(7)
O(5)-C(13)	1.436(7)
C(1)-C(2)	1.356(8)
C(1)-C(14)	1.455(8)
C(1)-C(11)	1.535(8)
C(2)-C(3)	1.469(8)
C(3)-C(4)	1.343(8)
C(3)-C(8)	1.501(9)
C(4)-C(15)	1.498(8)
C(4)-C(5)	1.502(8)
C(5)-C(6)	1.538(8)
C(6)-C(7)	1.539(7)
C(7)-C(8)	1.532(7)
C(8)-C(9)	1.531(7)
C(8)-C(16)	1.558(9)
C(9)-C(10)	1.536(8)
C(10)-C(11)	1.549(9)
C(11)-C(17)	1.541(8)
C(11)-C(12)	1.570(8)
C(12)-C(13)	1.532(8)
C(12)-C(18)	1.546(7)
C(13)-C(14)	1.517(8)
C(18)-C(19)	1.526(8)
C(18)-C(20)	1.532(8)
C(2)-O(4)-C(15)	109.9(4)
C(21)-O(5)-C(13)	113.3(4)
C(2)-C(1)-C(14)	123.4(5)
C(2)-C(1)-C(11)	125.9(5)
C(14)-C(1)-C(11)	110.6(5)
C(1)-C(2)-O(4)	120.3(5)
C(1)-C(2)-C(3)	132.1(5)
O(4)-C(2)-C(3)	107.6(5)
C(4)-C(3)-C(2)	108.2(5)
C(4)-C(3)-C(8)	123.4(5)
C(2)-C(3)-C(8)	128.1(5)
C(3)-C(4)-C(15)	110.3(5)
C(3)-C(4)-C(5)	125.9(5)
C(15)-C(4)-C(5)	123.6(5)
O(1)-C(5)-C(4)	106.2(5)
O(1)-C(5)-C(6)	111.9(5)
C(4)-C(5)-C(6)	110.0(5)
C(5)-C(6)-C(7)	111.5(5)
C(8)-C(7)-C(6)	112.7(4)
C(3)-C(8)-C(7)	108.4(5)
C(3)-C(8)-C(9)	115.7(5)
C(7)-C(8)-C(9)	108.0(4)
C(3)-C(8)-C(16)	106.9(5)
C(7)-C(8)-C(16)	108.4(5)
C(9)-C(8)-C(16)	109.1(5)
C(8)-C(9)-C(10)	115.9(5)

C(9)-C(10)-C(11)	116.2(6)
C(1)-C(11)-C(17)	108.8(5)
C(1)-C(11)-C(10)	113.6(5)
C(17)-C(11)-C(10)	110.9(5)
C(1)-C(11)-C(12)	101.8(4)
C(17)-C(11)-C(12)	111.8(5)
C(10)-C(11)-C(12)	109.6(5)
C(13)-C(12)-C(18)	112.4(5)
C(13)-C(12)-C(11)	104.6(5)
C(18)-C(12)-C(11)	120.1(5)
O(5)-C(13)-C(14)	108.1(5)
O(5)-C(13)-C(12)	109.0(4)
C(14)-C(13)-C(12)	105.3(5)
O(3)-C(14)-C(1)	129.3(5)
O(3)-C(14)-C(13)	123.0(5)
C(1)-C(14)-C(13)	107.7(5)
O(2)-C(15)-O(4)	109.8(4)
O(2)-C(15)-C(4)	113.4(5)
O(4)-C(15)-C(4)	103.1(4)
C(19)-C(18)-C(20)	109.9(5)
C(19)-C(18)-C(12)	114.5(5)
C(20)-C(18)-C(12)	108.9(5)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	16(2)	25(3)	34(3)	1(3)	2(2)	-6(2)
O(2)	27(2)	26(3)	17(2)	2(2)	0(2)	14(2)
O(3)	18(2)	35(3)	18(3)	1(2)	8(2)	6(2)
O(4)	12(2)	26(3)	10(2)	-5(2)	-2(2)	1(2)
O(5)	27(3)	16(3)	20(2)	1(2)	5(2)	5(2)
C(1)	16(4)	13(4)	15(3)	3(3)	-3(3)	1(3)
C(2)	23(4)	6(4)	16(4)	8(4)	8(3)	4(3)
C(3)	13(4)	9(4)	11(3)	3(3)	3(3)	-1(3)
C(4)	21(4)	13(4)	13(3)	7(3)	5(3)	5(3)
C(5)	11(4)	28(5)	17(3)	2(4)	0(3)	-2(3)
C(6)	11(3)	27(5)	25(3)	9(4)	0(3)	6(4)
C(7)	20(4)	23(4)	20(3)	-1(4)	2(3)	5(3)
C(8)	13(4)	17(4)	18(3)	0(4)	3(3)	-3(3)
C(9)	14(4)	34(5)	22(4)	-8(4)	2(3)	6(4)
C(10)	25(4)	31(4)	12(3)	-5(4)	-3(3)	7(4)
C(11)	16(3)	14(4)	13(3)	0(3)	7(3)	-3(3)
C(12)	20(4)	15(4)	16(3)	3(3)	0(3)	-4(3)
C(13)	19(4)	16(4)	13(3)	1(4)	2(3)	1(3)
C(14)	22(4)	9(4)	18(4)	5(3)	6(3)	-2(3)
C(15)	20(4)	26(5)	8(4)	6(4)	-3(3)	-1(3)
C(16)	32(4)	10(4)	35(4)	-7(4)	8(3)	2(3)
C(17)	23(4)	24(4)	14(3)	1(3)	2(3)	-6(4)
C(18)	21(4)	12(4)	14(3)	-2(3)	-6(3)	-2(3)
C(19)	29(4)	44(5)	17(3)	-13(4)	-2(3)	-1(4)
C(20)	22(4)	27(4)	20(3)	-2(4)	-5(3)	-2(3)
C(21)	29(4)	24(5)	41(4)	2(4)	11(3)	19(4)

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

	x	y	z	U(eq)
H(1A)	4892	8196	10906	38
H(2A)	8184	10407	9215	35
H(5A)	6098	10145	9913	23
H(6A)	4955	11694	11254	25
H(6B)	6125	13036	10871	25
H(7A)	6321	12924	12588	25
H(7B)	6410	10450	12558	25
H(9A)	8492	10339	13508	28
H(9B)	8350	12784	13638	28
H(10A)	10493	12285	14075	27
H(10B)	10520	13063	12992	27
H(12A)	12718	11846	13224	21
H(13A)	14116	9629	12564	19
H(15A)	8292	6872	10066	22
H(16A)	9443	14152	11790	38
H(16B)	8169	15131	12213	38
H(16C)	8063	14187	11149	38
H(17A)	9637	7820	13509	30
H(17B)	10726	8251	14382	30
H(17C)	11073	6816	13503	30
H(18A)	13038	8673	14659	19
H(19A)	12999	11305	15826	45
H(19B)	11618	11224	15187	45
H(19C)	12667	12995	15001	45
H(20A)	15048	10399	15151	35
H(20B)	14811	11939	14254	35
H(20C)	15055	9524	14079	35
H(21A)	14305	4299	12876	46
H(21B)	15114	6290	12578	46
H(21C)	13847	5537	11911	46

Table 1. Crystal data and structure refinement for guanacastepene J.

Identification code	cr1157	
Empirical formula	C21 H28 O5	
Formula weight	360.43	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 12.092(2) Å	α= 90°.
	b = 6.0388(10) Å	β= 97.576(4)°.
	c = 12.899(2) Å	γ = 90°.
Volume	933.6(3) $Å^3$	
Z	2	
Density (calculated)	1.282 Mg/m^3	
Absorption coefficient	0.090 mm^{-1}	
F(000)	388	
Crystal size	0.40 x 0.04 x 0.02 mm^3	
Theta range for data collection	2.48 to 20.81°.	
Index ranges	-10<=h<=12, -5<=k<=6, -12<=l<=12	
Reflections collected	3258	
Independent reflections	1907 [R(int) = 0.0766]	
Completeness to theta = 20.81°	99.2 %	
Absorption correction	SADABS	
Max. and min. transmission	1 and 0.717500	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1907 / 1 / 235	
Goodness-of-fit on F^2	0.925	
Final R indices [I>2sigma(I)]	R1 = 0.0690, wR2 = 0.1461	
R indices (all data)	R1 = 0.1190, wR2 = 0.1803	
Absolute structure parameter	-4(4)	
Largest diff. peak and hole	0.220 and -0.240 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	3654(5)	8643(10)	7916(4)	38(2)
O(2)	5955(5)	6571(10)	6475(4)	29(2)
O(3)	3012(5)	7270(11)	1152(5)	45(2)
O(4)	4862(5)	6539(10)	2906(4)	32(2)
O(5)	4777(4)	6355(9)	4978(4)	21(1)
C(1)	3164(6)	6152(14)	3707(6)	17(2)
C(2)	3626(6)	6068(14)	4720(6)	21(2)
C(3)	3156(6)	5794(14)	5696(6)	22(2)
C(4)	3966(6)	6252(14)	6479(6)	20(2)
C(5)	3793(7)	6385(16)	7625(6)	33(2)
C(6)	2734(7)	5147(16)	7795(6)	36(3)
C(7)	1776(7)	5586(15)	6915(6)	29(3)
C(8)	2026(7)	4843(14)	5832(6)	22(2)
C(9)	1121(6)	5709(13)	5008(5)	20(2)
C(10)	1155(7)	4908(14)	3889(5)	22(2)
C(11)	1956(6)	6026(13)	3219(5)	19(2)
C(12)	2021(7)	4750(15)	2167(6)	24(2)
C(13)	3146(7)	5439(16)	1842(6)	32(3)
C(14)	3863(7)	6083(15)	2846(6)	25(2)
C(15)	5022(8)	6454(14)	6060(6)	22(2)
C(16)	2129(7)	2326(14)	5783(7)	30(2)
C(17)	1575(7)	8468(13)	2988(6)	28(2)
C(18)	1086(7)	4839(17)	1265(6)	32(3)
C(19)	-49(8)	4064(18)	1515(7)	46(3)
C(20)	1381(7)	3425(17)	362(6)	47(3)
C(21)	3914(9)	7500(20)	552(7)	72(4)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene J.

O(1)-C(5)	1.430(11)
O(2)-C(15)	1.185(9)
O(3)-C(13)	1.415(10)
O(3)-C(21)	1.424(10)
O(4)-C(14)	1.232(9)
O(5)-C(15)	1.389(9)
O(5)-C(2)	1.398(9)
C(1)-C(2)	1.352(9)
C(1)-C(14)	1.482(10)
C(1)-C(11)	1.515(10)
C(2)-C(3)	1.458(10)
C(3)-C(4)	1.339(10)
C(3)-C(8)	1.513(11)
C(4)-C(15)	1.456(10)
C(4)-C(5)	1.522(10)
C(5)-C(6)	1.523(11)
C(6)-C(7)	1.534(11)
C(7)-C(8)	1.535(10)
C(8)-C(9)	1.515(10)
C(8)-C(16)	1.527(11)
C(9)-C(10)	1.528(10)
C(10)-C(11)	1.538(10)
C(11)-C(17)	1.562(11)
C(11)-C(12)	1.571(10)
C(12)-C(18)	1.512(11)
C(12)-C(13)	1.533(11)
C(13)-C(14)	1.511(11)
C(18)-C(19)	1.525(12)
C(18)-C(20)	1.523(11)
C(13)-O(3)-C(21)	112.7(7)
C(15)-O(5)-C(2)	108.6(6)
C(2)-C(1)-C(14)	121.3(7)
C(2)-C(1)-C(11)	130.8(6)
C(14)-C(1)-C(11)	107.5(6)
C(1)-C(2)-O(5)	119.8(6)
C(1)-C(2)-C(3)	132.9(7)
O(5)-C(2)-C(3)	107.3(6)
C(4)-C(3)-C(2)	107.4(7)
C(4)-C(3)-C(8)	124.9(7)
C(2)-C(3)-C(8)	127.1(7)
C(3)-C(4)-C(15)	109.1(7)
C(3)-C(4)-C(5)	124.2(7)
C(15)-C(4)-C(5)	126.5(7)
O(1)-C(5)-C(4)	110.0(7)
O(1)-C(5)-C(6)	107.5(7)
C(4)-C(5)-C(6)	109.8(7)
C(5)-C(6)-C(7)	112.1(7)
C(8)-C(7)-C(6)	113.7(7)
C(9)-C(8)-C(3)	111.6(6)
C(9)-C(8)-C(16)	111.7(7)
C(3)-C(8)-C(16)	107.0(7)
C(9)-C(8)-C(7)	109.0(7)
C(3)-C(8)-C(7)	106.5(7)
C(16)-C(8)-C(7)	110.8(7)
C(8)-C(9)-C(10)	116.5(6)

C(9)-C(10)-C(11)	119.3(7)
C(1)-C(11)-C(10)	115.6(6)
C(1)-C(11)-C(17)	106.0(6)
C(10)-C(11)-C(17)	109.3(6)
C(1)-C(11)-C(12)	103.2(6)
C(10)-C(11)-C(12)	112.2(6)
C(17)-C(11)-C(12)	110.2(6)
C(18)-C(12)-C(13)	112.3(6)
C(18)-C(12)-C(11)	122.0(7)
C(13)-C(12)-C(11)	104.5(6)
O(3)-C(13)-C(14)	110.1(7)
O(3)-C(13)-C(12)	110.6(7)
C(14)-C(13)-C(12)	105.4(6)
O(4)-C(14)-C(1)	126.8(7)
O(4)-C(14)-C(13)	123.9(7)
C(1)-C(14)-C(13)	109.3(7)
O(2)-C(15)-O(5)	121.4(7)
O(2)-C(15)-C(4)	131.8(8)
O(5)-C(15)-C(4)	106.7(7)
C(12)-C(18)-C(19)	115.4(7)
C(12)-C(18)-C(20)	110.0(7)
C(19)-C(18)-C(20)	107.3(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for guanacastepene J. 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)	53(5)	38(4)	24(3)	-6(3)	11(3)	-10(4)
O(2)	20(4)	29(4)	35(4)	-3(3)	-8(3)	-1(3)
O(3)	51(5)	58(5)	25(4)	12(4)	7(3)	-26(4)
O(4)	29(4)	40(4)	27(3)	-4(3)	10(3)	-7(4)
O(5)	15(3)	24(4)	26(3)	-3(3)	8(3)	8(3)
C(1)	17(5)	17(5)	17(5)	2(5)	2(4)	-2(5)
C(2)	11(5)	21(5)	33(6)	-2(5)	6(4)	2(5)
C(3)	20(5)	22(6)	23(5)	13(5)	3(5)	1(5)
C(4)	17(5)	17(5)	23(5)	5(5)	-4(4)	-2(5)
C(5)	41(6)	39(6)	20(5)	-5(5)	4(4)	-7(6)
C(6)	32(6)	53(7)	24(5)	6(5)	4(5)	-18(5)
C(7)	28(6)	35(7)	25(5)	-10(5)	10(4)	-15(5)
C(8)	13(5)	32(6)	20(5)	9(5)	-1(4)	-3(5)
C(9)	17(5)	23(6)	20(5)	-9(4)	6(4)	1(4)
C(10)	25(6)	16(5)	24(5)	0(4)	-6(4)	4(5)
C(11)	23(5)	12(5)	20(5)	2(4)	-4(4)	-6(5)
C(12)	24(6)	24(5)	28(5)	2(4)	16(5)	7(5)
C(13)	28(6)	53(7)	15(5)	-1(5)	2(4)	0(5)
C(14)	25(6)	25(6)	23(5)	3(5)	-4(4)	-3(6)
C(15)	36(6)	9(5)	21(5)	3(5)	4(5)	1(6)
C(16)	24(6)	26(6)	41(6)	9(5)	8(4)	-10(5)
C(17)	28(6)	15(5)	36(5)	2(5)	-8(4)	-2(5)
C(18)	38(7)	41(6)	14(5)	9(5)	-11(5)	-6(5)
C(19)	43(7)	64(8)	27(5)	-2(5)	-7(5)	-8(6)
C(20)	47(7)	74(8)	17(5)	-10(6)	-11(5)	-27(7)
C(21)	74(9)	116(11)	27(6)	11(6)	2(6)	-39(8)

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

	x	y	z	U(eq)
H(1)	3675	9442	7404	57
H(5)	4436	5739	8063	40
H(6A)	2508	5601	8457	44
H(6B)	2889	3571	7833	44
H(7A)	1115	4818	7076	35
H(7B)	1612	7159	6892	35
H(9A)	1161	7313	5011	24
H(9B)	404	5303	5212	24
H(10A)	406	5044	3518	27
H(10B)	1333	3341	3922	27
H(12)	2102	3183	2360	29
H(13)	3483	4193	1512	38
H(16A)	1404	1669	5762	45
H(16B)	2603	1809	6390	45
H(16C)	2445	1918	5166	45
H(17A)	1510	9214	3635	41
H(17B)	864	8474	2556	41
H(17C)	2115	9216	2632	41
H(18)	1010	6376	1022	39
H(19A)	48	2811	1976	69
H(19B)	-507	3649	879	69
H(19C)	-403	5243	1846	69
H(20A)	2020	4043	98	70
H(20B)	761	3396	-185	70
H(20C)	1548	1944	605	70
H(21A)	4603	7599	1014	109
H(21B)	3811	8821	136	109
H(21C)	3935	6239	103	109

Table 1. Crystal data and structure refinement for guanacastepene K.

Identification code	jan20	
Empirical formula	C22 H28 O6	
Formula weight	388.44	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.900(2) Å	α= 90°.
	b = 13.294(2) Å	β= 90°.
	c = 13.404(2) Å	γ = 90°.
Volume	1942.4(5) $Å^3$	
Z	4	
Density (calculated)	1.328 Mg/m^3	
Absorption coefficient	0.096 mm^{-1}	
F(000)	832	
Crystal size	0.60 x 0.40 x 0.10 mm^3	
Theta range for data collection	2.16 to 28.32°.	
Index ranges	-13<=h<=14, -14<=k<=17, -11<=l<=17	
Reflections collected	12357	
Independent reflections	4499 [R(int) = 0.0534]	
Absorption correction	SADABS	
Max. and min. transmission	1 and 0.632196	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4499 / 0 / 365	
Goodness-of-fit on F^2	0.768	
Final R indices [I>2sigma(I)]	R1 = 0.0352, wR2 = 0.0682	
R indices (all data)	R1 = 0.0578, wR2 = 0.0727	
Absolute structure parameter	0.89(83)	
Largest diff. peak and hole	0.177 and -0.181 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	-3391(1)	-1362(1)	7885(1)	49(1)
O(2)	-6573(1)	-564(1)	9598(1)	56(1)
O(3)	1497(1)	204(1)	7408(1)	38(1)
O(4)	-927(1)	445(1)	6657(1)	37(1)
O(5)	-877(1)	-1862(1)	7098(1)	33(1)
O(6)	2570(1)	1462(1)	8101(1)	44(1)
C(1)	-1504(2)	-425(1)	8192(1)	24(1)
C(2)	-2868(2)	-371(1)	7912(1)	30(1)
C(3)	-3696(1)	218(1)	8597(1)	26(1)
C(4)	-4669(2)	-351(1)	8818(1)	32(1)
C(5)	-5680(2)	-28(2)	9465(1)	39(1)
C(6)	-5495(2)	977(2)	9949(2)	42(1)
C(7)	-4751(2)	1699(2)	9314(2)	39(1)
C(8)	-3498(2)	1278(1)	8948(1)	31(1)
C(9)	-2579(2)	1288(1)	9825(1)	30(1)
C(10)	-1256(2)	981(1)	9568(2)	28(1)
C(11)	-1020(2)	-122(1)	9247(1)	26(1)
C(12)	354(2)	-300(1)	8952(1)	27(1)
C(13)	485(2)	409(1)	8069(1)	30(1)
C(14)	-705(2)	200(1)	7503(1)	28(1)
C(15)	-4590(2)	-1348(2)	8308(2)	37(1)
C(16)	-3054(2)	1949(2)	8091(2)	40(1)
C(17)	-1483(2)	-799(2)	10087(2)	31(1)
C(18)	385(2)	-1377(1)	8519(1)	30(1)
C(19)	-927(2)	-1506(1)	8090(1)	26(1)
C(20)	818(2)	-2197(2)	9225(2)	43(1)
C(21)	2483(2)	811(2)	7489(2)	34(1)
C(22)	3413(2)	552(2)	6714(2)	53(1)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene K.

O(1)-C(15)	1.425(2)
O(1)-C(2)	1.436(2)
O(2)-C(5)	1.219(2)
O(3)-C(21)	1.349(2)
O(3)-C(13)	1.441(2)
O(4)-C(14)	1.204(2)
O(5)-C(19)	1.412(2)
O(6)-C(21)	1.196(2)
C(1)-C(14)	1.518(2)
C(1)-C(2)	1.536(2)
C(1)-C(11)	1.562(2)
C(1)-C(19)	1.574(2)
C(2)-C(3)	1.507(2)
C(3)-C(4)	1.335(2)
C(3)-C(8)	1.502(2)
C(4)-C(5)	1.467(3)
C(4)-C(15)	1.494(3)
C(5)-C(6)	1.499(3)
C(6)-C(7)	1.518(3)
C(7)-C(8)	1.555(3)
C(8)-C(16)	1.533(3)
C(8)-C(9)	1.545(2)
C(9)-C(10)	1.538(2)
C(10)-C(11)	1.549(2)
C(11)-C(17)	1.527(3)
C(11)-C(12)	1.568(2)
C(12)-C(13)	1.520(3)
C(12)-C(18)	1.545(2)
C(13)-C(14)	1.528(2)
C(18)-C(20)	1.518(3)
C(18)-C(19)	1.551(2)
C(21)-C(22)	1.492(3)
C(15)-O(1)-C(2)	110.02(13)
C(21)-O(3)-C(13)	116.54(15)
C(14)-C(1)-C(2)	112.37(14)
C(14)-C(1)-C(11)	102.51(13)
C(2)-C(1)-C(11)	122.41(14)
C(14)-C(1)-C(19)	102.60(13)
C(2)-C(1)-C(19)	114.07(13)
C(11)-C(1)-C(19)	100.39(12)
O(1)-C(2)-C(3)	104.72(14)
O(1)-C(2)-C(1)	110.34(14)
C(3)-C(2)-C(1)	117.10(14)
C(4)-C(3)-C(2)	108.5(2)
C(4)-C(3)-C(8)	125.2(2)
C(2)-C(3)-C(8)	126.32(15)
C(3)-C(4)-C(5)	124.2(2)
C(3)-C(4)-C(15)	110.8(2)
C(5)-C(4)-C(15)	125.0(2)
O(2)-C(5)-C(4)	121.0(2)
O(2)-C(5)-C(6)	124.4(2)
C(4)-C(5)-C(6)	114.5(2)
C(5)-C(6)-C(7)	113.2(2)
C(6)-C(7)-C(8)	114.7(2)
C(3)-C(8)-C(16)	110.9(2)

C(3)-C(8)-C(9)	109.90(14)
C(16)-C(8)-C(9)	111.1(2)
C(3)-C(8)-C(7)	108.10(15)
C(16)-C(8)-C(7)	107.7(2)
C(9)-C(8)-C(7)	109.03(15)
C(10)-C(9)-C(8)	115.8(2)
C(9)-C(10)-C(11)	117.95(14)
C(17)-C(11)-C(10)	107.39(15)
C(17)-C(11)-C(1)	113.81(15)
C(10)-C(11)-C(1)	116.09(14)
C(17)-C(11)-C(12)	114.33(15)
C(10)-C(11)-C(12)	111.82(13)
C(1)-C(11)-C(12)	93.14(13)
C(13)-C(12)-C(18)	106.27(15)
C(13)-C(12)-C(11)	101.06(13)
C(18)-C(12)-C(11)	104.83(14)
O(3)-C(13)-C(12)	115.66(14)
O(3)-C(13)-C(14)	108.01(13)
C(12)-C(13)-C(14)	101.21(14)
O(4)-C(14)-C(1)	127.3(2)
O(4)-C(14)-C(13)	126.1(2)
C(1)-C(14)-C(13)	106.48(14)
O(1)-C(15)-C(4)	104.27(15)
C(20)-C(18)-C(12)	116.0(2)
C(20)-C(18)-C(19)	116.0(2)
C(12)-C(18)-C(19)	102.82(13)
O(5)-C(19)-C(18)	110.50(14)
O(5)-C(19)-C(1)	113.75(14)
C(18)-C(19)-C(1)	103.56(13)
O(6)-C(21)-O(3)	123.5(2)
O(6)-C(21)-C(22)	126.2(2)
O(3)-C(21)-C(22)	110.4(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for guanacastepene K. 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)	26(1)	37(1)	82(1)	-22(1)	2(1)	-6(1)
O(2)	28(1)	70(1)	70(1)	4(1)	7(1)	-9(1)
O(3)	27(1)	45(1)	41(1)	-5(1)	9(1)	-7(1)
O(4)	39(1)	38(1)	34(1)	8(1)	1(1)	4(1)
O(5)	31(1)	31(1)	35(1)	-8(1)	1(1)	-3(1)
O(6)	25(1)	42(1)	66(1)	1(1)	-6(1)	-2(1)
C(1)	21(1)	23(1)	29(1)	-1(1)	-1(1)	0(1)
C(2)	25(1)	30(1)	35(1)	-3(1)	-4(1)	-1(1)
C(3)	22(1)	30(1)	28(1)	1(1)	-7(1)	4(1)
C(4)	24(1)	36(1)	35(1)	4(1)	-8(1)	2(1)
C(5)	23(1)	52(1)	40(1)	9(1)	-4(1)	2(1)
C(6)	24(1)	59(1)	41(1)	-4(1)	1(1)	11(1)
C(7)	29(1)	40(1)	49(1)	-6(1)	-5(1)	9(1)
C(8)	23(1)	31(1)	37(1)	-1(1)	-2(1)	3(1)
C(9)	25(1)	28(1)	37(1)	-8(1)	-2(1)	2(1)
C(10)	22(1)	29(1)	35(1)	-5(1)	-2(1)	-1(1)
C(11)	19(1)	26(1)	32(1)	-3(1)	-2(1)	-1(1)
C(12)	19(1)	33(1)	30(1)	-4(1)	-2(1)	0(1)
C(13)	24(1)	30(1)	38(1)	-5(1)	3(1)	-2(1)
C(14)	27(1)	22(1)	33(1)	-1(1)	1(1)	4(1)
C(15)	27(1)	36(1)	48(1)	6(1)	-8(1)	-7(1)
C(16)	39(1)	29(1)	51(1)	2(1)	-2(1)	4(1)
C(17)	30(1)	36(1)	27(1)	-2(1)	0(1)	3(1)
C(18)	24(1)	34(1)	31(1)	-1(1)	2(1)	3(1)
C(19)	29(1)	23(1)	28(1)	0(1)	2(1)	-1(1)
C(20)	45(1)	36(1)	49(2)	-2(1)	-8(1)	14(1)
C(21)	22(1)	41(1)	40(1)	15(1)	-3(1)	0(1)
C(22)	30(1)	84(2)	46(2)	13(1)	7(1)	1(1)

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

	x	y	z	U(eq)
H(5O)	-1494(20)	-2156(15)	6969(15)	44(6)
H(2)	-2928(15)	-73(12)	7213(13)	24(4)
H(6B)	-6283(20)	1243(16)	10106(15)	54(6)
H(6A)	-5102(18)	871(15)	10590(17)	49(6)
H(7B)	-5209(18)	1842(14)	8680(13)	39(5)
H(7A)	-4607(18)	2345(16)	9689(14)	46(6)
H(9B)	-2907(14)	861(13)	10425(13)	26(4)
H(9A)	-2541(13)	2002(12)	10074(10)	14(4)
H(10B)	-963(15)	1459(12)	9079(12)	22(4)
H(10A)	-794(15)	1054(12)	10199(12)	25(4)
H(12)	919(15)	-166(11)	9489(11)	16(4)
H(13)	494(14)	1101(12)	8248(11)	18(4)
H(15B)	-5195(16)	-1431(13)	7760(13)	31(5)
H(15A)	-4647(16)	-1930(13)	8750(12)	29(5)
H(16C)	-2268(20)	1733(15)	7802(15)	55(6)
H(16B)	-3683(19)	1974(15)	7479(15)	53(6)
H(16A)	-2963(18)	2628(16)	8284(14)	44(6)
H(17C)	-1105(15)	-620(12)	10688(14)	24(5)
H(17B)	-2353(17)	-731(13)	10177(13)	33(5)
H(17A)	-1372(18)	-1494(17)	9930(14)	45(6)
H(18)	928(16)	-1335(13)	7954(13)	29(5)
H(19)	-1393(14)	-1977(11)	8488(11)	14(4)
H(20C)	749(20)	-2838(17)	8971(15)	53(6)
H(20B)	418(23)	-2142(18)	9940(18)	73(8)
H(20A)	1667(26)	-2096(20)	9399(19)	85(9)
H(22C)	3155(22)	663(19)	6032(21)	79(9)
H(22B)	3635(26)	-153(22)	6693(21)	97(11)
H(22A)	4132(33)	871(24)	6839(23)	122(12)

Table 1. Crystal data and structure refinement for guanacastepene L.

Identification code	m	
Empirical formula	C20 H26 O6	
Formula weight	362.41	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.5008(6) Å	α= 90°.
	b = 11.7446(8) Å	β= 90°.
	c = 17.7091(12) Å	γ = 90°.
Volume	1768.0(2) $Å^3$	
Z	4	
Density (calculated)	1.361 Mg/m^3	
Absorption coefficient	0.100 mm^{-1}	
F(000)	776	
Crystal size	0.40 x 0.05 x 0.03 mm^3	
Theta range for data collection	2.30 to 23.25°.	
Index ranges	-9<=h<=8, -13<=k<=13, -19<=l<=19	
Reflections collected	11462	
Independent reflections	2530 [R(int) = 0.0718]	
Completeness to theta = 23.25°	99.8 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9970 and 0.7955	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2530 / 0 / 339	
Goodness-of-fit on F^2	1.015	
Final R indices [I>2sigma(I)]	R1 = 0.0470, wR2 = 0.0896	
R indices (all data)	R1 = 0.0611, wR2 = 0.0946	
Absolute structure parameter	1.9(14)	
Largest diff. peak and hole	0.148 and -0.156 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	9224(3)	8964(2)	8307(1)	22(1)
O(1W)	13493(4)	11915(3)	10430(2)	38(1)
O(2)	8067(3)	10674(2)	8184(1)	31(1)
O(3)	11317(3)	12143(2)	9107(1)	25(1)
O(4)	10374(3)	5080(2)	9559(1)	26(1)
O(5)	8423(3)	6677(2)	8588(1)	27(1)
C(1)	11054(4)	7504(3)	8607(2)	18(1)
C(2)	10779(4)	8578(3)	8408(2)	18(1)
C(3)	11806(4)	9570(3)	8348(2)	16(1)
C(4)	10894(4)	10500(3)	8321(2)	18(1)
C(5)	11446(4)	11714(3)	8343(2)	21(1)
C(6)	13151(4)	11775(3)	8105(2)	24(1)
C(7)	14128(4)	10809(3)	8436(2)	22(1)
C(8)	13569(4)	9607(3)	8210(2)	19(1)
C(9)	14516(4)	8726(3)	8657(2)	20(1)
C(10)	14104(4)	7472(3)	8538(2)	22(1)
C(11)	12604(4)	7039(3)	8921(2)	17(1)
C(12)	12433(4)	5730(3)	8766(2)	20(1)
C(13)	10691(4)	5472(3)	8801(2)	22(1)
C(14)	9843(4)	6582(3)	8654(2)	22(1)
C(15)	9259(4)	10134(3)	8274(2)	21(1)
C(16)	13793(5)	9404(4)	7357(2)	26(1)
C(17)	12567(5)	7352(3)	9762(2)	20(1)
C(18)	13119(4)	4831(3)	9306(2)	22(1)
C(19)	11833(4)	4726(3)	9901(2)	25(1)
C(20)	14773(5)	4960(4)	9618(2)	30(1)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene L.

O(1)-C(15)	1.376(4)
O(1)-C(2)	1.408(4)
O(2)-C(15)	1.207(4)
O(3)-C(5)	1.449(4)
O(4)-C(19)	1.441(4)
O(4)-C(13)	1.444(4)
O(5)-C(14)	1.218(4)
C(1)-C(2)	1.330(5)
C(1)-C(14)	1.497(5)
C(1)-C(11)	1.531(5)
C(2)-C(3)	1.459(4)
C(3)-C(4)	1.341(4)
C(3)-C(8)	1.519(5)
C(4)-C(15)	1.457(5)
C(4)-C(5)	1.502(5)
C(5)-C(6)	1.511(5)
C(6)-C(7)	1.523(5)
C(7)-C(8)	1.542(5)
C(8)-C(9)	1.532(5)
C(8)-C(16)	1.541(4)
C(9)-C(10)	1.529(5)
C(10)-C(11)	1.531(5)
C(11)-C(17)	1.535(4)
C(11)-C(12)	1.568(4)
C(12)-C(13)	1.512(5)
C(12)-C(18)	1.539(4)
C(13)-C(14)	1.512(5)
C(18)-C(20)	1.518(6)
C(18)-C(19)	1.523(5)
C(15)-O(1)-C(2)	107.8(3)
C(19)-O(4)-C(13)	108.8(3)
C(2)-C(1)-C(14)	125.5(3)
C(2)-C(1)-C(11)	125.9(3)
C(14)-C(1)-C(11)	108.2(3)
C(1)-C(2)-O(1)	120.2(3)
C(1)-C(2)-C(3)	132.1(3)
O(1)-C(2)-C(3)	107.2(3)
C(4)-C(3)-C(2)	107.8(3)
C(4)-C(3)-C(8)	122.8(3)
C(2)-C(3)-C(8)	128.7(3)
C(3)-C(4)-C(15)	108.3(3)
C(3)-C(4)-C(5)	126.3(3)
C(15)-C(4)-C(5)	125.5(3)
O(3)-C(5)-C(4)	109.3(3)
O(3)-C(5)-C(6)	108.5(3)
C(4)-C(5)-C(6)	109.7(3)
C(5)-C(6)-C(7)	112.4(3)
C(6)-C(7)-C(8)	114.5(3)
C(3)-C(8)-C(9)	114.6(3)
C(3)-C(8)-C(7)	106.8(3)
C(9)-C(8)-C(7)	108.8(3)
C(3)-C(8)-C(16)	105.9(3)
C(9)-C(8)-C(16)	109.7(3)
C(7)-C(8)-C(16)	110.9(3)
C(10)-C(9)-C(8)	117.3(3)

C(9)-C(10)-C(11)	116.7(3)
C(1)-C(11)-C(10)	116.0(3)
C(1)-C(11)-C(17)	104.5(3)
C(10)-C(11)-C(17)	111.5(3)
C(1)-C(11)-C(12)	101.9(3)
C(10)-C(11)-C(12)	109.0(3)
C(17)-C(11)-C(12)	113.7(3)
C(13)-C(12)-C(18)	102.0(3)
C(13)-C(12)-C(11)	106.3(3)
C(18)-C(12)-C(11)	121.9(3)
O(4)-C(13)-C(14)	110.3(3)
O(4)-C(13)-C(12)	106.5(3)
C(14)-C(13)-C(12)	106.7(3)
O(5)-C(14)-C(1)	127.5(3)
O(5)-C(14)-C(13)	124.6(3)
C(1)-C(14)-C(13)	107.8(3)
O(2)-C(15)-O(1)	120.8(3)
O(2)-C(15)-C(4)	130.8(3)
O(1)-C(15)-C(4)	108.2(3)
C(20)-C(18)-C(19)	114.9(3)
C(20)-C(18)-C(12)	120.6(3)
C(19)-C(18)-C(12)	102.3(3)
O(4)-C(19)-C(18)	107.6(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for guanacastepene L. 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)	11(1)	24(1)	32(1)	4(1)	-3(1)	-1(1)
O(1W)	32(2)	35(2)	49(2)	-11(1)	-11(2)	5(2)
O(2)	18(2)	33(2)	42(2)	7(1)	-2(1)	5(1)
O(3)	24(2)	27(1)	26(1)	-5(1)	3(1)	2(1)
O(4)	23(2)	28(1)	27(1)	6(1)	2(1)	0(1)
O(5)	17(2)	33(2)	32(1)	0(1)	-4(1)	-7(1)
C(1)	18(2)	21(2)	14(2)	-4(1)	0(1)	1(2)
C(2)	11(2)	30(2)	12(2)	-4(1)	-1(1)	4(2)
C(3)	17(2)	18(2)	13(2)	-2(1)	-1(1)	-1(2)
C(4)	13(2)	24(2)	16(2)	-1(2)	-1(1)	-2(2)
C(5)	20(2)	24(2)	20(2)	5(2)	-2(2)	6(2)
C(6)	22(2)	21(2)	27(2)	2(2)	5(2)	1(2)
C(7)	12(2)	29(2)	25(2)	3(2)	2(2)	-2(2)
C(8)	15(2)	21(2)	20(2)	2(2)	1(2)	-2(2)
C(9)	12(2)	25(2)	24(2)	4(2)	-1(2)	-3(2)
C(10)	18(2)	26(2)	24(2)	3(2)	1(2)	5(2)
C(11)	15(2)	21(2)	16(2)	-2(1)	3(2)	0(2)
C(12)	21(2)	23(2)	15(2)	-3(1)	2(2)	0(2)
C(13)	31(2)	17(2)	17(2)	-3(2)	1(2)	-2(2)
C(14)	22(2)	29(2)	14(2)	-3(2)	-2(2)	-6(2)
C(15)	17(2)	25(2)	21(2)	3(2)	2(2)	2(2)
C(16)	25(2)	28(2)	25(2)	4(2)	9(2)	4(2)
C(17)	21(2)	19(2)	22(2)	-2(2)	-2(2)	-1(2)
C(18)	31(2)	17(2)	19(2)	-2(2)	4(2)	5(2)
C(19)	29(2)	18(2)	29(2)	3(2)	-2(2)	-1(2)
C(20)	35(3)	30(2)	27(2)	7(2)	1(2)	6(2)

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

	x	y	z	U(eq)
H(6B)	13570(30)	12530(30)	8254(15)	11(8)
H(20C)	14880(40)	5580(30)	9980(20)	39(11)
H(17C)	12520(40)	8150(30)	9849(18)	28(10)
H(2W)	12960(50)	11990(30)	9990(30)	52(14)
H(17B)	13500(40)	7070(30)	10054(18)	22(9)
H(19B)	11760(40)	3920(30)	10017(18)	29(10)
H(17A)	11610(40)	7030(20)	10053(16)	17(8)
H(9B)	15580(40)	8830(20)	8474(17)	18(9)
H(9A)	14500(30)	8940(20)	9200(18)	14(8)
H(19A)	12070(30)	5250(20)	10327(15)	0(7)
H(20B)	15140(40)	4220(30)	9927(18)	25(9)
H(1W)	13980(60)	11270(40)	10400(30)	70(18)
H(10B)	14980(40)	7050(30)	8779(17)	15(9)
H(10A)	14030(30)	7290(20)	7981(17)	11(8)
H(7B)	15220(40)	10880(30)	8281(19)	30(10)
H(16C)	13210(40)	9960(30)	7050(20)	40(11)
H(18)	13130(30)	4170(30)	9005(16)	6(8)
H(13)	10370(30)	4870(20)	8443(15)	6(7)
H(12)	12820(30)	5670(20)	8256(17)	15(8)
H(5A)	10790(40)	12170(30)	8023(16)	15(8)
H(7A)	14150(40)	10840(30)	8940(20)	26(10)
H(16B)	13300(40)	8580(30)	7195(18)	32(10)
H(20A)	15520(50)	5090(30)	9260(20)	50(13)
H(6A)	13180(40)	11800(30)	7560(20)	38(11)
H(16A)	14870(50)	9450(40)	7220(20)	43(12)
H(3O)	10420(60)	12320(40)	9250(30)	86(17)

Table 1. Crystal data and structure refinement for *p*-bromobenzoyl guanacastepene L.

Identification code	sean14	
Empirical formula	C57 H53 Br2 O12	
Formula weight	1089.81	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.475(17) Å	α= 90°.
	b = 18.70(3) Å	β= 90°.
	c = 31.82(6) Å	γ = 90°.
Volume	5043(17) $Å^3$	
Z	4	
Density (calculated)	1.435 Mg/m^3	
Absorption coefficient	1.672 mm^{-1}	
F(000)	2244	
Crystal size	0.4 x 0.3 x 0.02 mm^3	
Theta range for data collection	1.26 to 15.85°.	
Index ranges	-6<=h<=6, -13<=k<=14, -24<=l<=24	
Reflections collected	7864	
Independent reflections	2387 [R(int) = 0.0986]	
Completeness to theta = 15.85°	98.7 %	
Absorption correction	SADABS	
Max. and min. transmission	1 and 0.119462	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2387 / 0 / 296	
Goodness-of-fit on F^2	1.102	
Final R indices [I>2sigma(I)]	R1 = 0.1072, wR2 = 0.2633	
R indices (all data)	R1 = 0.1290, wR2 = 0.2801	
Absolute structure parameter	0.16(5)	
Largest diff. peak and hole	1.349 and -0.659 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Br(1)	593(10)	8395(3)	8504(2)	183(3)
O(1)	3395(16)	11253(8)	11204(4)	9(4)
O(2)	4580(20)	11362(8)	10555(5)	27(5)
O(3)	1277(17)	10985(9)	9950(5)	19(5)
O(4)	1709(19)	11630(11)	9385(5)	39(6)
O(5)	2000(20)	10219(10)	12662(5)	39(6)
O(6)	4036(18)	11068(8)	12044(4)	14(4)
C(1)	1430(30)	11046(13)	11736(7)	12(7)
C(2)	1800(30)	11235(13)	11337(7)	4(7)
C(3)	770(30)	11383(12)	10975(7)	13(7)
C(4)	1740(30)	11453(12)	10630(7)	5(7)
C(5)	1230(30)	11633(14)	10208(8)	22(8)
C(6)	-530(20)	11934(13)	10192(7)	12(7)
C(7)	-1500(30)	11550(12)	10498(6)	9(7)
C(8)	-940(30)	11595(13)	10974(7)	14(7)
C(9)	-1970(30)	11056(13)	11250(7)	9(7)
C(10)	-1670(30)	11129(13)	11710(6)	9(7)
C(11)	-100(30)	10783(14)	11904(8)	24(8)
C(12)	30(30)	11028(14)	12374(7)	19(8)
C(13)	1690(30)	10930(14)	12456(8)	22(8)
C(14)	2600(30)	10991(12)	12073(7)	3(7)
C(15)	3350(30)	11365(14)	10744(8)	27(8)
C(16)	-990(30)	12367(13)	11153(7)	22(8)
C(17)	-110(30)	9973(11)	11803(7)	6(7)
C(18)	-810(30)	10528(14)	12709(8)	31(8)
C(19)	510(30)	9963(15)	12749(9)	45(9)
C(20)	-2410(30)	10264(16)	12672(9)	48(9)
C(21)	1430(30)	11065(18)	9523(9)	39(9)
C(22)	1100(40)	10416(18)	9311(10)	46(10)
C(23)	1680(30)	10393(18)	8900(9)	46(9)
C(24)	1480(40)	9830(20)	8656(12)	77(12)
C(25)	720(50)	9270(20)	8839(15)	111(15)
C(26)	130(50)	9250(30)	9250(15)	118(16)
C(27)	270(40)	9850(20)	9491(13)	81(13)
Br(1')	5842(6)	3864(2)	5405(1)	107(2)
O(1')	3453(19)	6915(9)	7763(5)	25(5)
O(2')	4790(20)	7197(9)	7162(5)	31(5)
O(3')	2113(19)	6426(9)	6524(5)	28(5)
O(4')	2240(20)	6997(11)	5918(6)	39(6)
O(5')	2250(20)	5837(11)	9197(6)	64(7)
O(6')	4070(30)	6723(11)	8597(6)	64(7)
C(1')	1530(30)	6534(14)	8252(8)	20(8)
C(2')	1880(30)	6790(12)	7862(7)	3(7)
C(3')	1010(30)	6867(12)	7487(7)	1(7)
C(4')	1980(30)	6945(14)	7175(8)	29(8)
C(5')	1500(30)	7003(16)	6732(8)	34(9)
C(6')	-310(30)	7100(14)	6665(8)	27(8)
C(7')	-1190(30)	6655(16)	6988(8)	38(9)
C(8')	-810(30)	6839(13)	7456(7)	16(7)
C(9')	-1700(30)	6359(15)	7747(7)	30(9)
C(10')	-1490(30)	6492(14)	8211(7)	21(8)
C(11')	40(30)	6242(15)	8417(8)	29(8)

C(12')	80(30)	6448(15)	8900(7)	26(9)
C(13')	1720(30)	6534(17)	9016(9)	46(10)
C(14')	2700(40)	6601(15)	8623(9)	38(9)
C(15')	3580(30)	7055(14)	7331(8)	21(8)
C(16')	-1390(30)	7641(14)	7538(8)	38(9)
C(17')	180(30)	5453(14)	8334(8)	33(9)
C(18')	-710(30)	5956(15)	9238(9)	43(9)
C(19')	770(30)	5498(17)	9315(9)	54(9)
C(20')	-2190(30)	5575(16)	9161(9)	50(10)
C(21')	2480(40)	6506(19)	6099(10)	48(10)
C(22')	3250(40)	5874(18)	5957(10)	57(10)
C(23')	3980(30)	5880(17)	5551(9)	48(10)
C(24')	4760(30)	5305(17)	5385(10)	59(10)
C(25')	4820(30)	4675(16)	5626(9)	35(9)
C(26')	3970(40)	4610(20)	6000(10)	66(11)
C(27')	3230(40)	5210(20)	6160(11)	66(12)
C(1S)	6780(90)	2250(40)	4760(20)	190(30)
C(2S)	5790(80)	2160(30)	4926(19)	160(20)
C(3S)	4720(60)	1810(30)	5324(15)	144(18)

Table 3. Bond lengths [Å] and angles [°] for *p*-bromobenzoyl guanacastepene L.

Br(1)-C(25)	1.95(5)
O(1)-C(2)	1.42(2)
O(1)-C(15)	1.48(3)
O(2)-C(15)	1.20(2)
O(3)-C(21)	1.37(3)
O(3)-C(5)	1.46(3)
O(4)-C(21)	1.17(3)
O(5)-C(19)	1.38(3)
O(5)-C(13)	1.51(3)
O(6)-C(14)	1.23(2)
C(1)-C(2)	1.36(3)
C(1)-C(14)	1.47(3)
C(1)-C(11)	1.48(3)
C(2)-C(3)	1.47(3)
C(3)-C(4)	1.38(3)
C(3)-C(8)	1.50(3)
C(4)-C(15)	1.42(3)
C(4)-C(5)	1.45(3)
C(5)-C(6)	1.60(3)
C(6)-C(7)	1.46(3)
C(7)-C(8)	1.59(3)
C(8)-C(16)	1.55(3)
C(8)-C(9)	1.60(3)
C(9)-C(10)	1.49(3)
C(10)-C(11)	1.61(3)
C(11)-C(17)	1.55(3)
C(11)-C(12)	1.57(3)
C(12)-C(13)	1.44(3)
C(12)-C(18)	1.59(3)
C(13)-C(14)	1.45(3)
C(18)-C(20)	1.45(3)
C(18)-C(19)	1.54(3)
C(21)-C(22)	1.42(4)
C(22)-C(23)	1.40(4)
C(22)-C(27)	1.39(4)
C(23)-C(24)	1.32(4)
C(24)-C(25)	1.37(5)
C(25)-C(26)	1.40(5)
C(26)-C(27)	1.36(5)
Br(1')-C(25')	1.88(3)
O(1')-C(2')	1.39(2)
O(1')-C(15')	1.40(3)
O(2')-C(15')	1.19(2)
O(3')-C(5')	1.37(3)
O(3')-C(21')	1.40(3)
O(4')-C(21')	1.10(3)
O(5')-C(13')	1.50(3)
O(5')-C(19')	1.46(3)
O(6')-C(14')	1.18(3)
C(1')-C(2')	1.36(3)
C(1')-C(11')	1.47(3)
C(1')-C(14')	1.55(4)
C(2')-C(3')	1.41(3)
C(3')-C(4')	1.30(3)
C(3')-C(8')	1.54(3)
C(4')-C(15')	1.46(3)

C(4')-C(5')	1.47(3)
C(5')-C(6')	1.56(4)
C(6')-C(7')	1.52(3)
C(7')-C(8')	1.56(3)
C(8')-C(9')	1.49(3)
C(8')-C(16')	1.60(3)
C(9')-C(10')	1.51(3)
C(10')-C(11')	1.53(3)
C(11')-C(17')	1.50(3)
C(11')-C(12')	1.58(3)
C(12')-C(13')	1.44(3)
C(12')-C(18')	1.57(3)
C(13')-C(14')	1.51(4)
C(18')-C(20')	1.46(4)
C(18')-C(19')	1.54(4)
C(21')-C(22')	1.43(4)
C(22')-C(27')	1.39(4)
C(22')-C(23')	1.43(4)
C(23')-C(24')	1.37(3)
C(24')-C(25')	1.41(4)
C(25')-C(26')	1.40(4)
C(26')-C(27')	1.38(4)
C(1S)-C(2S)	1.00(8)
C(2S)-C(3S)	1.69(7)

C(2)-O(1)-C(15)	106.0(17)
C(21)-O(3)-C(5)	118(2)
C(19)-O(5)-C(13)	103.4(18)
C(2)-C(1)-C(14)	123(2)
C(2)-C(1)-C(11)	129(2)
C(14)-C(1)-C(11)	107.8(19)
C(1)-C(2)-O(1)	121(2)
C(1)-C(2)-C(3)	130(2)
O(1)-C(2)-C(3)	109.1(19)
C(4)-C(3)-C(2)	106.8(19)
C(4)-C(3)-C(8)	123(2)
C(2)-C(3)-C(8)	129(2)
C(3)-C(4)-C(15)	111(2)
C(3)-C(4)-C(5)	126(2)
C(15)-C(4)-C(5)	123(2)
O(3)-C(5)-C(4)	108.5(19)
O(3)-C(5)-C(6)	107.5(19)
C(4)-C(5)-C(6)	113(2)
C(7)-C(6)-C(5)	109.3(19)
C(6)-C(7)-C(8)	116.1(19)
C(16)-C(8)-C(9)	111.6(19)
C(16)-C(8)-C(7)	112.9(19)
C(9)-C(8)-C(7)	109.1(18)
C(16)-C(8)-C(3)	105.9(19)
C(9)-C(8)-C(3)	111.0(19)
C(7)-C(8)-C(3)	106.2(19)
C(10)-C(9)-C(8)	113.0(19)
C(9)-C(10)-C(11)	118.6(19)
C(1)-C(11)-C(17)	105(2)
C(1)-C(11)-C(12)	101(2)
C(17)-C(11)-C(12)	119(2)
C(1)-C(11)-C(10)	116.8(19)
C(17)-C(11)-C(10)	108(2)

C(12)-C(11)-C(10)	107.9(19)
C(13)-C(12)-C(18)	104(2)
C(13)-C(12)-C(11)	102(2)
C(18)-C(12)-C(11)	116(2)
C(12)-C(13)-C(14)	111(2)
C(12)-C(13)-O(5)	111(2)
C(14)-C(13)-O(5)	110.0(19)
O(6)-C(14)-C(13)	127(2)
O(6)-C(14)-C(1)	128(2)
C(13)-C(14)-C(1)	104.8(19)
O(2)-C(15)-C(4)	135(2)
O(2)-C(15)-O(1)	118(2)
C(4)-C(15)-O(1)	107(2)
C(20)-C(18)-C(12)	124(2)
C(20)-C(18)-C(19)	117(2)
C(12)-C(18)-C(19)	98(2)
O(5)-C(19)-C(18)	114(2)
O(4)-C(21)-C(22)	129(3)
O(4)-C(21)-O(3)	119(3)
C(22)-C(21)-O(3)	111(3)
C(21)-C(22)-C(23)	114(3)
C(21)-C(22)-C(27)	124(3)
C(23)-C(22)-C(27)	123(3)
C(24)-C(23)-C(22)	122(3)
C(23)-C(24)-C(25)	115(4)
C(24)-C(25)-C(26)	126(5)
C(24)-C(25)-Br(1)	116(4)
C(26)-C(25)-Br(1)	118(4)
C(27)-C(26)-C(25)	118(5)
C(26)-C(27)-C(22)	116(4)
C(2')-O(1')-C(15')	109.0(18)
C(5')-O(3')-C(21')	118(2)
C(13')-O(5')-C(19')	103(2)
C(2')-C(1')-C(11')	130(2)
C(2')-C(1')-C(14')	122(2)
C(11')-C(1')-C(14')	108(2)
O(1')-C(2')-C(3')	107(2)
O(1')-C(2')-C(1')	118(2)
C(3')-C(2')-C(1')	134(2)
C(4')-C(3')-C(2')	109(2)
C(4')-C(3')-C(8')	126(2)
C(2')-C(3')-C(8')	125(2)
C(3')-C(4')-C(15')	110(2)
C(3')-C(4')-C(5')	125(2)
C(15')-C(4')-C(5')	125(2)
O(3')-C(5')-C(4')	108(2)
O(3')-C(5')-C(6')	113(2)
C(4')-C(5')-C(6')	114(2)
C(7')-C(6')-C(5')	109(2)
C(8')-C(7')-C(6')	115(2)
C(3')-C(8')-C(7')	106.1(19)
C(3')-C(8')-C(9')	119(2)
C(7')-C(8')-C(9')	110.7(19)
C(3')-C(8')-C(16')	105.5(18)
C(7')-C(8')-C(16')	107(2)
C(9')-C(8')-C(16')	108(2)
C(10')-C(9')-C(8')	117(2)
C(9')-C(10')-C(11')	118(2)

C(1')-C(11')-C(17')	104(2)
C(1')-C(11')-C(10')	118(2)
C(17')-C(11')-C(10')	107(2)
C(1')-C(11')-C(12')	104(2)
C(17')-C(11')-C(12')	114(2)
C(10')-C(11')-C(12')	111(2)
C(13')-C(12')-C(18')	108(2)
C(13')-C(12')-C(11')	107(2)
C(18')-C(12')-C(11')	121(2)
C(12')-C(13')-C(14')	109(2)
C(12')-C(13')-O(5')	107(2)
C(14')-C(13')-O(5')	103(2)
O(6')-C(14')-C(13')	128(3)
O(6')-C(14')-C(1')	126(3)
C(13')-C(14')-C(1')	106(2)
O(2')-C(15')-O(1')	123(2)
O(2')-C(15')-C(4')	133(2)
O(1')-C(15')-C(4')	104(2)
C(20')-C(18')-C(19')	117(3)
C(20')-C(18')-C(12')	123(2)
C(19')-C(18')-C(12')	95(2)
O(5')-C(19')-C(18')	115(2)
O(4')-C(21')-O(3')	124(3)
O(4')-C(21')-C(22')	127(3)
O(3')-C(21')-C(22')	109(3)
C(27')-C(22')-C(21')	125(3)
C(27')-C(22')-C(23')	116(3)
C(21')-C(22')-C(23')	119(3)
C(24')-C(23')-C(22')	123(3)
C(25')-C(24')-C(23')	118(3)
C(24')-C(25')-C(26')	121(3)
C(24')-C(25')-Br(1')	119(2)
C(26')-C(25')-Br(1')	119(2)
C(27')-C(26')-C(25')	119(3)
C(22')-C(27')-C(26')	123(3)
C(1S)-C(2S)-C(3S)	154(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for *p*-bromobenzoyl guanacastepene L. 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}
Br(1)	401(10)	58(4)	91(4)	-24(3)	-17(5)	-44(5)
Br(1')	197(5)	70(3)	54(3)	-13(3)	20(3)	35(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for *p*-bromobenzoyl guanacastepene L.

	x	y	z	U(eq)
H(5A)	1961	11997	10086	26
H(6A)	-535	12451	10258	14
H(6B)	-976	11869	9907	14
H(7A)	-1534	11040	10416	11
H(7B)	-2591	11737	10481	11
H(9A)	-3100	11144	11193	11
H(9B)	-1725	10560	11164	11
H(10A)	-2587	10917	11859	11
H(10B)	-1665	11646	11777	11
H(12A)	-287	11539	12409	22
H(13A)	2039	11315	12653	27
H(16A)	-609	12365	11443	33
H(16B)	-2083	12542	11147	33
H(16C)	-325	12680	10982	33
H(17A)	861	9753	11910	9
H(17B)	-166	9905	11498	9
H(17C)	-1025	9749	11936	9
H(18A)	-781	10803	12979	38
H(19A)	505	9770	13038	54
H(19B)	279	9564	12554	54
H(20A)	-3143	10670	12653	72
H(20B)	-2675	9976	12920	72
H(20C)	-2506	9970	12419	72
H(23A)	2237	10795	8794	55
H(24A)	1840	9819	8374	92
H(26A)	-365	8833	9358	142
H(27A)	-166	9879	9766	97
H(5'A)	2028	7439	6616	40
H(6'A)	-598	7611	6695	32
H(6'B)	-604	6944	6378	32
H(7'A)	-2338	6719	6943	46
H(7'B)	-944	6145	6939	46
H(9'A)	-2833	6400	7680	37
H(9'B)	-1378	5860	7688	37
H(10C)	-2380	6258	8359	26
H(10D)	-1591	7013	8259	26
H(12B)	-424	6930	8925	31
H(13B)	1882	6943	9214	55
H(16D)	-1169	7775	7830	56
H(16E)	-2532	7672	7487	56
H(16F)	-839	7968	7348	56
H(17D)	100	5365	8031	50
H(17E)	-678	5201	8479	50
H(17F)	1196	5280	8438	50
H(18B)	-875	6255	9495	52
H(19C)	718	5030	9430	64
H(20D)	-2484	5302	9412	75
H(20E)	-2058	5248	8923	75
H(20F)	-3028	5921	9096	75
H(23B)	3928	6305	5389	57
H(24B)	5250	5330	5116	70
H(26B)	3895	4168	6142	80

H(27B)	2677	5174	6420	79

Table 1. Crystal data and structure refinement for guanacastepene M.

Identification code	sean28	
Empirical formula	C20 H22 O5	
Formula weight	342.38	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.4212(10) Å	α= 90°.
	b = 10.4740(13) Å	β= 90°.
	c = 18.314(2) Å	γ = 90°.
Volume	1615.4(3) $Å^3$	
Z	4	
Density (calculated)	1.408 Mg/m^3	
Absorption coefficient	0.101 mm^{-1}	
F(000)	728	
Crystal size	0.40 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.95 to 24.71°.	
Index ranges	-9<=h<=9, -12<=k<=12, -20<=l<=21	
Reflections collected	8509	
Independent reflections	2755 [R(int) = 0.0446]	
Completeness to theta = 24.71°	99.7 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9900 and 0.844384	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2755 / 0 / 314	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0408, wR2 = 0.0792	
R indices (all data)	R1 = 0.0615, wR2 = 0.0868	
Absolute structure parameter	-0.2(12)	
Largest diff. peak and hole	0.151 and -0.161 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	5986(2)	1994(2)	8370(1)	27(1)
O(2)	7360(2)	330(2)	7917(1)	37(1)
O(3)	5057(2)	-1976(2)	8015(1)	35(1)
O(4)	4360(2)	5861(2)	9966(1)	47(1)
O(5)	6565(2)	4389(2)	8944(1)	45(1)
C(1)	3985(3)	3365(2)	8828(1)	24(1)
C(2)	4386(3)	2264(2)	8505(1)	22(1)
C(3)	3462(3)	1149(2)	8285(1)	23(1)
C(4)	4505(3)	217(2)	8112(1)	24(1)
C(5)	4066(3)	-1130(2)	7992(1)	26(1)
C(6)	2322(3)	-1353(2)	7878(2)	31(1)
C(7)	1288(3)	-417(2)	8311(2)	30(1)
C(8)	1690(3)	1002(2)	8178(1)	24(1)
C(9)	662(3)	1805(3)	8695(2)	30(1)
C(10)	929(3)	3249(3)	8698(2)	28(1)
C(11)	2368(3)	3723(2)	9132(1)	26(1)
C(12)	2435(3)	5230(2)	9093(2)	30(1)
C(13)	4163(4)	5588(3)	9203(2)	35(1)
C(14)	5129(3)	4422(3)	8992(2)	32(1)
C(15)	6105(3)	753(2)	8111(1)	28(1)
C(16)	1369(3)	1378(3)	7379(2)	31(1)
C(17)	2352(4)	3192(3)	9916(1)	32(1)
C(18)	1614(4)	6081(3)	9660(2)	39(1)
C(19)	2818(4)	6144(3)	10280(2)	47(1)
C(20)	-85(4)	5775(3)	9906(2)	44(1)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene M.

O(1)-C(15)	1.388(3)
O(1)-C(2)	1.398(3)
O(2)-C(15)	1.200(3)
O(3)-C(5)	1.218(3)
O(4)-C(13)	1.436(3)
O(4)-C(19)	1.450(4)
O(5)-C(14)	1.213(3)
C(1)-C(2)	1.339(3)
C(1)-C(14)	1.499(4)
C(1)-C(11)	1.519(3)
C(2)-C(3)	1.460(3)
C(3)-C(4)	1.350(3)
C(3)-C(8)	1.513(3)
C(4)-C(15)	1.460(3)
C(4)-C(5)	1.475(3)
C(5)-C(6)	1.503(4)
C(6)-C(7)	1.533(4)
C(7)-C(8)	1.544(4)
C(8)-C(9)	1.534(4)
C(8)-C(16)	1.539(4)
C(9)-C(10)	1.529(4)
C(10)-C(11)	1.532(4)
C(11)-C(17)	1.539(3)
C(11)-C(12)	1.581(3)
C(12)-C(13)	1.517(4)
C(12)-C(18)	1.533(4)
C(13)-C(14)	1.518(4)
C(18)-C(19)	1.524(4)
C(18)-C(20)	1.534(4)
C(15)-O(1)-C(2)	108.63(17)
C(13)-O(4)-C(19)	108.8(2)
C(2)-C(1)-C(14)	124.2(2)
C(2)-C(1)-C(11)	127.0(2)
C(14)-C(1)-C(11)	108.7(2)
C(1)-C(2)-O(1)	119.7(2)
C(1)-C(2)-C(3)	132.5(2)
O(1)-C(2)-C(3)	107.63(19)
C(4)-C(3)-C(2)	107.3(2)
C(4)-C(3)-C(8)	122.5(2)
C(2)-C(3)-C(8)	130.0(2)
C(3)-C(4)-C(15)	108.8(2)
C(3)-C(4)-C(5)	124.3(2)
C(15)-C(4)-C(5)	126.8(2)
O(3)-C(5)-C(4)	121.3(2)
O(3)-C(5)-C(6)	124.1(2)
C(4)-C(5)-C(6)	114.5(2)
C(5)-C(6)-C(7)	112.5(2)
C(6)-C(7)-C(8)	114.2(2)
C(3)-C(8)-C(9)	114.9(2)
C(3)-C(8)-C(16)	105.7(2)
C(9)-C(8)-C(16)	110.3(2)
C(3)-C(8)-C(7)	107.1(2)
C(9)-C(8)-C(7)	107.9(2)
C(16)-C(8)-C(7)	111.0(2)
C(10)-C(9)-C(8)	117.5(2)

C(9)-C(10)-C(11)	116.0(2)
C(1)-C(11)-C(10)	116.0(2)
C(1)-C(11)-C(17)	105.1(2)
C(10)-C(11)-C(17)	111.1(2)
C(1)-C(11)-C(12)	101.4(2)
C(10)-C(11)-C(12)	109.1(2)
C(17)-C(11)-C(12)	113.8(2)
C(13)-C(12)-C(18)	101.5(2)
C(13)-C(12)-C(11)	106.0(2)
C(18)-C(12)-C(11)	122.2(2)
O(4)-C(13)-C(12)	106.8(2)
O(4)-C(13)-C(14)	110.2(2)
C(12)-C(13)-C(14)	106.3(2)
O(5)-C(14)-C(1)	127.3(3)
O(5)-C(14)-C(13)	125.2(3)
C(1)-C(14)-C(13)	107.5(2)
O(2)-C(15)-O(1)	120.7(2)
O(2)-C(15)-C(4)	132.2(2)
O(1)-C(15)-C(4)	107.0(2)
C(19)-C(18)-C(12)	103.3(2)
C(19)-C(18)-C(20)	114.3(3)
C(12)-C(18)-C(20)	119.8(3)
O(4)-C(19)-C(18)	107.0(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for guanacastepene M. 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)	16(1)	32(1)	33(1)	2(1)	-1(1)	-2(1)
O(2)	17(1)	50(1)	46(1)	-1(1)	2(1)	4(1)
O(3)	33(1)	33(1)	39(1)	0(1)	-1(1)	9(1)
O(4)	54(1)	50(1)	38(1)	-13(1)	-3(1)	-14(1)
O(5)	29(1)	41(1)	63(2)	-2(1)	-2(1)	-12(1)
C(1)	21(1)	26(1)	26(1)	5(1)	-4(1)	-2(1)
C(2)	14(1)	30(1)	23(1)	6(1)	-2(1)	-2(1)
C(3)	19(1)	30(1)	19(1)	3(1)	-1(1)	-1(1)
C(4)	17(1)	30(1)	25(2)	-1(1)	0(1)	-1(1)
C(5)	24(1)	31(1)	24(1)	1(1)	3(1)	4(1)
C(6)	23(1)	24(1)	45(2)	-3(1)	3(1)	-3(1)
C(7)	18(2)	31(2)	41(2)	-5(1)	1(1)	-5(1)
C(8)	15(1)	28(1)	28(2)	-2(1)	0(1)	-1(1)
C(9)	18(2)	34(2)	37(2)	-7(1)	1(1)	-3(1)
C(10)	22(1)	32(1)	31(2)	-5(1)	-2(1)	5(1)
C(11)	26(1)	27(1)	26(2)	1(1)	0(1)	-1(1)
C(12)	38(2)	26(1)	26(2)	1(1)	-2(1)	-3(1)
C(13)	44(2)	27(2)	34(2)	0(1)	2(1)	-12(2)
C(14)	32(2)	36(2)	29(2)	6(1)	-2(1)	-9(1)
C(15)	19(1)	37(2)	27(2)	5(1)	-1(1)	2(1)
C(16)	21(2)	37(2)	35(2)	-5(1)	-4(1)	1(1)
C(17)	32(2)	32(2)	31(2)	3(1)	-6(1)	-5(2)
C(18)	54(2)	26(2)	37(2)	-7(1)	5(1)	0(2)
C(19)	57(2)	43(2)	41(2)	-13(2)	5(2)	-17(2)
C(20)	46(2)	40(2)	48(2)	-10(2)	11(2)	8(2)

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

	x	y	z	U(eq)
H(6B)	2010(30)	-2250(20)	8009(13)	27(6)
H(6A)	2170(30)	-1280(20)	7327(16)	46(9)
H(7B)	220(30)	-550(20)	8145(13)	26(7)
H(7A)	1390(30)	-600(20)	8869(15)	30(7)
H(9B)	780(30)	1430(20)	9207(15)	37(7)
H(9)	-390(30)	1670(30)	8547(13)	32(7)
H(10B)	1080(20)	3532(19)	8199(13)	17(6)
H(10A)	-60(30)	3660(20)	8922(12)	23(6)
H(12)	2050(30)	5440(20)	8604(13)	21(6)
H(13)	4560(30)	6310(20)	8917(13)	31(7)
H(16C)	1650(30)	2250(20)	7265(13)	28(7)
H(16B)	300(30)	1300(20)	7287(14)	33(7)
H(16A)	2010(30)	840(20)	7024(14)	37(7)
H(17C)	3210(30)	3560(30)	10210(15)	45(8)
H(17B)	2520(30)	2300(20)	9913(13)	27(7)
H(17A)	1220(30)	3310(20)	10128(12)	25(6)
H(18)	1580(30)	6930(30)	9446(13)	29(7)
H(19A)	2820(30)	7050(30)	10523(16)	57(9)
H(19)	2570(40)	5460(30)	10661(17)	66(10)
H(20C)	-120(40)	4940(30)	10135(16)	53(9)
H(20B)	-490(30)	6440(30)	10263(15)	47(8)
H(20A)	-780(40)	5620(30)	9520(20)	79(13)

Table 1. Crystal data and structure refinement for guanacastepene N.

Identification code	sean-m05	
Empirical formula	C22 H28 O6	
Formula weight	388.44	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 12.120(2) Å	α= 90°.
	b = 6.0521(7) Å	β= 100.190(5)°.
	c = 13.459(2) Å	γ = 90°.
Volume	971.6(3) $Å^3$	
Z	2	
Density (calculated)	1.328 Mg/m^3	
Absorption coefficient	0.096 mm^{-1}	
F(000)	416	
Crystal size	0.80 x 0.10 x 0.01 mm^3	
Theta range for data collection	2.49 to 21.96°.	
Index ranges	-9<=h<=12, -5<=k<=5, -6<=l<=14	
Reflections collected	1884	
Independent reflections	1670 [R(int) = 0.0275]	
Completeness to theta = 21.96°	78.3 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9990 and 0.781517	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1670 / 1 / 254	
Goodness-of-fit on F^2	1.004	
Final R indices [I>2sigma(I)]	R1 = 0.0527, wR2 = 0.0894	
R indices (all data)	R1 = 0.0854, wR2 = 0.1015	
Absolute structure parameter	-2(3)	
Largest diff. peak and hole	0.162 and -0.161 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	5188(4)	1341(8)	-94(3)	23(1)
O(2)	3950(4)	1625(7)	-1550(3)	32(1)
O(3)	6231(4)	3659(8)	-2888(3)	40(1)
O(4)	7050(4)	2734(8)	3545(3)	31(1)
O(5)	5932(5)	1266(12)	4530(4)	66(2)
O(6)	5184(4)	1556(8)	1922(3)	28(1)
C(1)	6832(5)	1183(12)	1135(4)	16(2)
C(2)	6349(5)	1064(12)	164(5)	18(2)
C(3)	6789(5)	798(11)	-782(4)	20(2)
C(4)	5943(6)	1210(12)	-1543(4)	24(2)
C(5)	6077(5)	1385(15)	-2636(5)	34(2)
C(6)	7101(6)	159(11)	-2810(5)	36(2)
C(7)	8105(6)	578(11)	-1967(4)	31(2)
C(8)	7893(6)	-126(12)	-892(5)	24(2)
C(9)	8876(5)	718(11)	-102(4)	25(2)
C(10)	8857(5)	-11(11)	993(4)	24(2)
C(11)	8094(5)	1233(12)	1585(4)	18(2)
C(12)	8103(5)	131(10)	2659(4)	25(2)
C(13)	6980(5)	740(12)	2958(4)	25(2)
C(14)	6188(6)	1234(12)	1962(4)	21(2)
C(15)	4917(6)	1436(12)	-1139(5)	25(2)
C(16)	7817(6)	-2637(11)	-855(5)	28(2)
C(17)	8427(5)	3665(11)	1719(4)	28(2)
C(18)	9110(5)	574(11)	3526(4)	30(2)
C(19)	10255(6)	-81(12)	3299(5)	45(2)
C(20)	8913(6)	-711(12)	4463(5)	47(2)
C(21)	6454(6)	2818(16)	4304(5)	35(2)
C(22)	6546(6)	5017(12)	4808(5)	43(3)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene N.

O(1)-C(15)	1.388(7)
O(1)-C(2)	1.399(7)
O(2)-C(15)	1.210(7)
O(3)-C(5)	1.438(9)
O(4)-C(21)	1.353(8)
O(4)-C(13)	1.436(8)
O(5)-C(21)	1.202(9)
O(6)-C(14)	1.224(7)
C(1)-C(2)	1.337(7)
C(1)-C(14)	1.469(9)
C(1)-C(11)	1.542(8)
C(2)-C(3)	1.474(8)
C(3)-C(4)	1.338(7)
C(3)-C(8)	1.482(9)
C(4)-C(15)	1.449(9)
C(4)-C(5)	1.512(8)
C(5)-C(6)	1.500(10)
C(6)-C(7)	1.531(8)
C(7)-C(8)	1.572(9)
C(8)-C(16)	1.524(8)
C(8)-C(9)	1.537(8)
C(9)-C(10)	1.542(8)
C(10)-C(11)	1.523(9)
C(11)-C(17)	1.529(9)
C(11)-C(12)	1.590(8)
C(12)-C(13)	1.531(9)
C(12)-C(18)	1.555(8)
C(13)-C(14)	1.534(7)
C(18)-C(20)	1.535(9)
C(18)-C(19)	1.526(10)
C(21)-C(22)	1.489(9)
C(15)-O(1)-C(2)	107.7(5)
C(21)-O(4)-C(13)	117.3(6)
C(2)-C(1)-C(14)	122.9(5)
C(2)-C(1)-C(11)	128.1(5)
C(14)-C(1)-C(11)	109.0(5)
C(1)-C(2)-O(1)	118.9(5)
C(1)-C(2)-C(3)	133.5(5)
O(1)-C(2)-C(3)	107.5(5)
C(4)-C(3)-C(2)	107.2(6)
C(4)-C(3)-C(8)	125.2(6)
C(2)-C(3)-C(8)	126.8(5)
C(3)-C(4)-C(15)	108.8(6)
C(3)-C(4)-C(5)	124.0(7)
C(15)-C(4)-C(5)	127.3(5)
O(3)-C(5)-C(6)	106.9(6)
O(3)-C(5)-C(4)	109.7(6)
C(6)-C(5)-C(4)	110.5(6)
C(5)-C(6)-C(7)	112.0(6)
C(6)-C(7)-C(8)	113.5(6)
C(3)-C(8)-C(16)	108.2(7)
C(3)-C(8)-C(9)	114.1(6)
C(16)-C(8)-C(9)	110.6(6)
C(3)-C(8)-C(7)	106.7(5)
C(16)-C(8)-C(7)	108.7(6)

C(9)-C(8)-C(7)	108.3(7)
C(8)-C(9)-C(10)	115.2(6)
C(11)-C(10)-C(9)	118.2(5)
C(10)-C(11)-C(17)	111.4(5)
C(10)-C(11)-C(1)	115.9(5)
C(17)-C(11)-C(1)	106.7(6)
C(10)-C(11)-C(12)	111.2(5)
C(17)-C(11)-C(12)	109.7(5)
C(1)-C(11)-C(12)	101.3(5)
C(13)-C(12)-C(18)	112.1(5)
C(13)-C(12)-C(11)	106.0(5)
C(18)-C(12)-C(11)	119.2(6)
O(4)-C(13)-C(12)	112.2(5)
O(4)-C(13)-C(14)	106.5(5)
C(12)-C(13)-C(14)	105.4(5)
O(6)-C(14)-C(1)	128.8(5)
O(6)-C(14)-C(13)	122.3(6)
C(1)-C(14)-C(13)	108.9(6)
O(2)-C(15)-O(1)	120.2(7)
O(2)-C(15)-C(4)	131.6(7)
O(1)-C(15)-C(4)	108.2(5)
C(20)-C(18)-C(19)	108.2(5)
C(20)-C(18)-C(12)	108.3(6)
C(19)-C(18)-C(12)	115.2(5)
O(5)-C(21)-O(4)	122.5(8)
O(5)-C(21)-C(22)	125.7(7)
O(4)-C(21)-C(22)	111.8(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for guanacastepene N. 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)	12(3)	27(3)	29(3)	3(2)	3(2)	-2(3)
O(2)	13(3)	32(4)	45(3)	2(3)	-5(2)	0(3)
O(3)	42(3)	38(4)	45(3)	15(3)	21(3)	14(3)
O(4)	31(3)	31(3)	31(3)	-3(3)	8(2)	0(3)
O(5)	81(5)	55(5)	74(4)	-6(3)	47(3)	-26(4)
O(6)	17(3)	30(4)	37(3)	2(2)	5(2)	1(3)
C(1)	12(4)	7(4)	32(4)	9(4)	8(3)	-1(4)
C(2)	13(4)	9(4)	34(4)	-1(4)	7(4)	4(4)
C(3)	14(4)	15(5)	31(4)	0(4)	4(3)	6(3)
C(4)	35(5)	16(4)	21(4)	-2(4)	1(3)	-2(4)
C(5)	21(4)	41(6)	38(4)	-9(5)	3(3)	1(5)
C(6)	34(5)	37(6)	35(4)	7(4)	4(4)	2(4)
C(7)	27(5)	41(6)	27(4)	7(4)	8(3)	15(4)
C(8)	23(5)	19(5)	28(4)	2(4)	-4(3)	1(4)
C(9)	9(4)	22(5)	44(4)	-4(4)	6(3)	-2(3)
C(10)	22(4)	21(5)	28(4)	-1(3)	-1(3)	2(4)
C(11)	9(4)	13(5)	33(4)	-2(4)	8(3)	-4(4)
C(12)	25(5)	16(5)	31(4)	0(3)	-3(4)	-9(4)
C(13)	24(5)	27(6)	25(4)	-3(4)	4(3)	1(4)
C(14)	24(5)	7(4)	28(4)	3(4)	-5(3)	-12(4)
C(15)	21(5)	6(5)	47(5)	-2(4)	4(4)	5(4)
C(16)	23(4)	17(7)	42(4)	1(3)	1(3)	5(3)
C(17)	25(4)	25(5)	32(4)	4(4)	2(3)	-1(4)
C(18)	28(5)	25(5)	31(4)	-6(4)	-9(3)	3(4)
C(19)	29(5)	61(6)	37(5)	-5(4)	-11(4)	10(4)
C(20)	40(6)	60(7)	33(5)	9(4)	-10(4)	-1(5)
C(21)	31(5)	46(8)	30(5)	-9(5)	13(4)	8(5)
C(22)	35(5)	50(7)	49(5)	-4(4)	18(4)	10(4)

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

	x	y	z	U(eq)
H(3A)	5816	4463	-2603	60
H(5A)	5398	774	-3083	40
H(6A)	7294	627	-3463	43
H(6B)	6937	-1444	-2851	43
H(7A)	8293	2170	-1955	37
H(7B)	8760	-247	-2121	37
H(9A)	8879	2352	-125	30
H(9B)	9585	198	-293	30
H(10A)	8642	-1590	978	29
H(10B)	9632	93	1375	29
H(12A)	8083	-1502	2545	30
H(13A)	6688	-509	3324	31
H(16A)	7673	-3094	-192	42
H(16B)	8526	-3284	-969	42
H(16C)	7205	-3148	-1380	42
H(17A)	8437	4329	1056	42
H(17B)	9174	3780	2136	42
H(17C)	7883	4447	2049	42
H(18A)	9125	2187	3689	36
H(19A)	10403	742	2709	67
H(19B)	10262	-1669	3158	67
H(19C)	10835	263	3883	67
H(20A)	9544	-463	5016	70
H(20B)	8851	-2291	4305	70
H(20C)	8219	-197	4666	70
H(22A)	5950(20)	5266(17)	5062(11)	65
H(22B)	6616(7)	6040(40)	4368(18)	65
H(22C)	7130(20)	5031(12)	5290(20)	65

Table 1. Crystal data and structure refinement for guanacastepene O.

Identification code	seana18	
Empirical formula	C22 H28 O6	
Formula weight	388.44	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2	
Unit cell dimensions	a = 25.506(7) Å	α= 90°.
	b = 6.2372(17) Å	β= 99.953(10)°.
	c = 12.602(3) Å	γ = 90°.
Volume	1974.6(9) $Å^3$	
Z	4	
Density (calculated)	1.307 Mg/m^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	832	
Crystal size	0.40 x 0.05 x 0.03 mm^3	
Theta range for data collection	2.50 to 21.97°.	
Index ranges	-14<=h<=26, -6<=k<=5, -13<=l<=13	
Reflections collected	2735	
Independent reflections	1914 [R(int) = 0.0380]	
Completeness to theta = 21.97°	95.5 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9972 and 0.744944	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1914 / 1 / 354	
Goodness-of-fit on F^2	0.979	
Final R indices [I>2sigma(I)]	R1 = 0.0469, wR2 = 0.0847	
R indices (all data)	R1 = 0.0776, wR2 = 0.0961	
Absolute structure parameter	2(2)	
Largest diff. peak and hole	0.184 and -0.183 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	2568(1)	3594(6)	4938(3)	23(1)
O(3)	4208(2)	1698(7)	4882(4)	34(1)
O(2)	3184(1)	3385(6)	6464(3)	26(1)
O(4)	739(1)	4870(6)	2527(3)	29(1)
O(6)	1483(1)	3617(7)	4324(3)	28(1)
O(5)	272(2)	1835(9)	2684(4)	58(2)
C(1)	2135(2)	3755(10)	3129(4)	21(1)
C(2)	2580(2)	3946(9)	3852(4)	19(1)
C(3)	3137(2)	4331(8)	3753(4)	17(2)
C(4)	3440(2)	3935(9)	4702(5)	23(2)
C(5)	4041(2)	3893(11)	4954(5)	28(2)
C(6)	4254(3)	5164(13)	4083(5)	32(2)
C(7)	3943(2)	4737(13)	2941(6)	26(2)
C(8)	3346(2)	5315(10)	2805(5)	24(2)
C(9)	3063(2)	4555(12)	1716(5)	27(2)
C(10)	2464(2)	5145(12)	1412(6)	29(2)
C(11)	2069(2)	3721(10)	1895(4)	20(1)
C(12)	1494(2)	4660(10)	1548(5)	25(2)
C(13)	1197(2)	3617(13)	2386(5)	27(2)
C(14)	1595(2)	3605(10)	3421(5)	21(1)
C(15)	3091(2)	3578(10)	5503(5)	22(1)
C(16)	3292(3)	7768(11)	2911(6)	34(2)
C(17)	2101(3)	1415(10)	1517(5)	26(2)
C(18)	1227(2)	4509(10)	366(5)	29(2)
C(19)	838(3)	2696(14)	95(7)	49(2)
C(20)	957(3)	6633(12)	0(6)	65(2)
C(21)	299(2)	3743(15)	2699(5)	37(2)
C(22)	-116(3)	5273(14)	2950(7)	43(2)

Table 3. Bond lengths [Å] and angles [°] for guanacastepene O.

O(1)-C(2)	1.392(6)
O(1)-C(15)	1.401(6)
O(3)-C(5)	1.441(7)
O(2)-C(15)	1.199(6)
O(4)-C(21)	1.373(7)
O(4)-C(13)	1.441(6)
O(6)-C(14)	1.219(6)
O(5)-C(21)	1.192(8)
C(1)-C(2)	1.333(7)
C(1)-C(14)	1.489(7)
C(1)-C(11)	1.536(7)
C(2)-C(3)	1.468(7)
C(3)-C(4)	1.329(7)
C(3)-C(8)	1.518(7)
C(4)-C(15)	1.473(7)
C(4)-C(5)	1.512(7)
C(5)-C(6)	1.527(8)
C(6)-C(7)	1.541(9)
C(7)-C(8)	1.546(8)
C(8)-C(9)	1.512(9)
C(8)-C(16)	1.544(9)
C(9)-C(10)	1.553(8)
C(10)-C(11)	1.545(8)
C(11)-C(17)	1.521(8)
C(11)-C(12)	1.571(7)
C(12)-C(18)	1.531(8)
C(12)-C(13)	1.545(8)
C(13)-C(14)	1.509(7)
C(18)-C(19)	1.504(9)
C(18)-C(20)	1.527(9)
C(21)-C(22)	1.499(10)
C(2)-O(1)-C(15)	108.6(4)
C(21)-O(4)-C(13)	116.3(5)
C(2)-C(1)-C(14)	123.5(5)
C(2)-C(1)-C(11)	128.6(4)
C(14)-C(1)-C(11)	107.9(4)
C(1)-C(2)-O(1)	119.8(4)
C(1)-C(2)-C(3)	132.8(5)
O(1)-C(2)-C(3)	107.2(4)
C(4)-C(3)-C(2)	108.2(4)
C(4)-C(3)-C(8)	123.7(5)
C(2)-C(3)-C(8)	127.5(5)
C(3)-C(4)-C(15)	108.7(5)
C(3)-C(4)-C(5)	127.0(5)
C(15)-C(4)-C(5)	124.3(5)
O(3)-C(5)-C(4)	107.7(5)
O(3)-C(5)-C(6)	107.6(5)
C(4)-C(5)-C(6)	108.2(5)
C(5)-C(6)-C(7)	113.1(6)
C(6)-C(7)-C(8)	113.6(5)
C(9)-C(8)-C(3)	114.2(5)
C(9)-C(8)-C(16)	110.7(6)
C(3)-C(8)-C(16)	106.5(5)
C(9)-C(8)-C(7)	109.5(5)
C(3)-C(8)-C(7)	106.9(5)

C(16)-C(8)-C(7)	108.8(6)
C(8)-C(9)-C(10)	116.3(5)
C(11)-C(10)-C(9)	116.6(5)
C(17)-C(11)-C(1)	109.1(5)
C(17)-C(11)-C(10)	110.3(5)
C(1)-C(11)-C(10)	115.3(5)
C(17)-C(11)-C(12)	111.3(5)
C(1)-C(11)-C(12)	102.0(4)
C(10)-C(11)-C(12)	108.5(5)
C(18)-C(12)-C(13)	116.8(5)
C(18)-C(12)-C(11)	119.0(5)
C(13)-C(12)-C(11)	101.4(4)
O(4)-C(13)-C(14)	109.5(5)
O(4)-C(13)-C(12)	111.0(5)
C(14)-C(13)-C(12)	104.9(5)
O(6)-C(14)-C(1)	127.3(5)
O(6)-C(14)-C(13)	125.2(4)
C(1)-C(14)-C(13)	107.4(5)
O(2)-C(15)-O(1)	121.2(5)
O(2)-C(15)-C(4)	132.2(5)
O(1)-C(15)-C(4)	106.6(5)
C(19)-C(18)-C(20)	109.8(5)
C(19)-C(18)-C(12)	115.6(6)
C(20)-C(18)-C(12)	110.0(5)
O(5)-C(21)-O(4)	123.8(6)
O(5)-C(21)-C(22)	126.6(6)
O(4)-C(21)-C(22)	109.5(7)

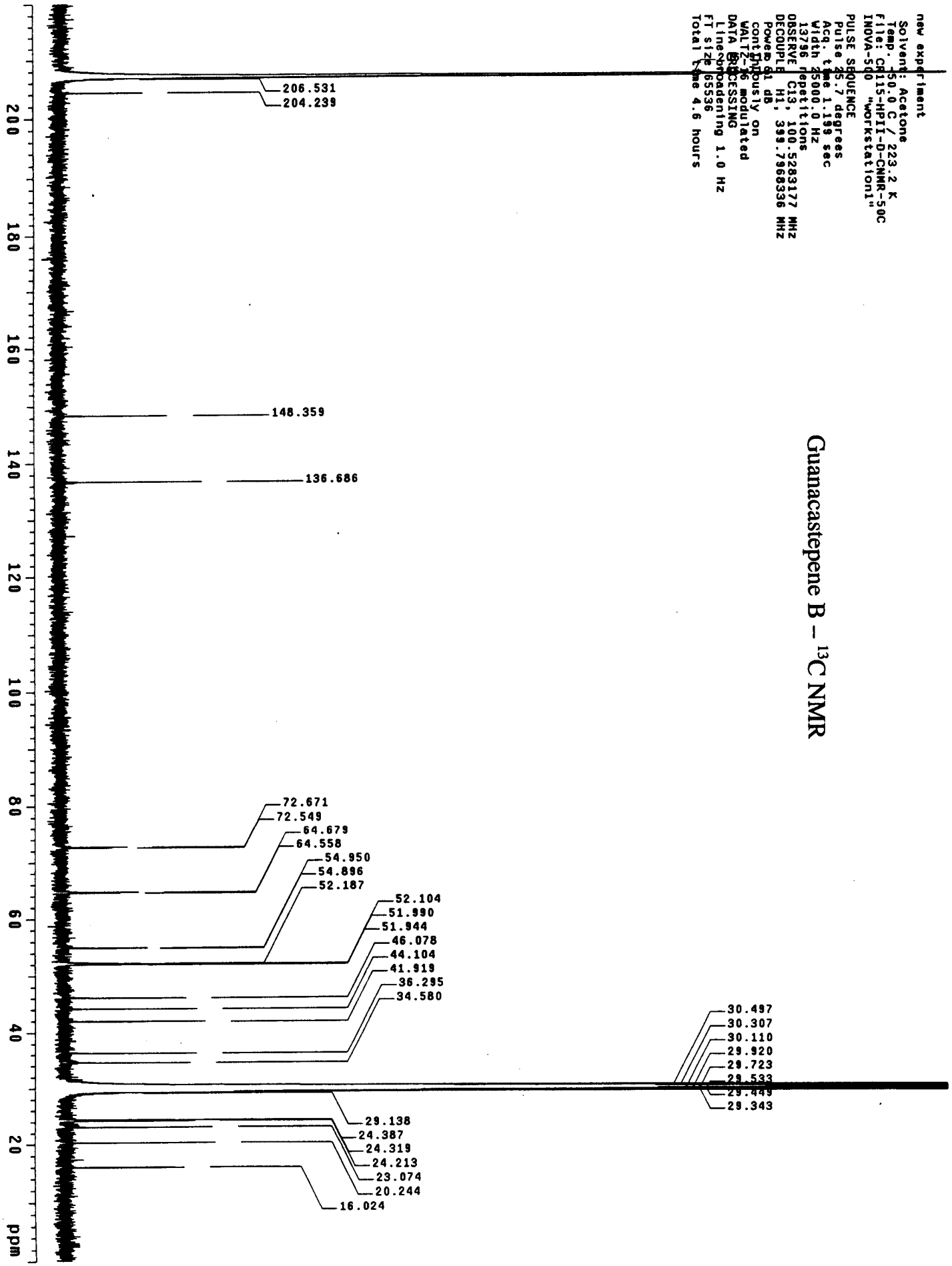
Symmetry transformations used to generate equivalent atoms:

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

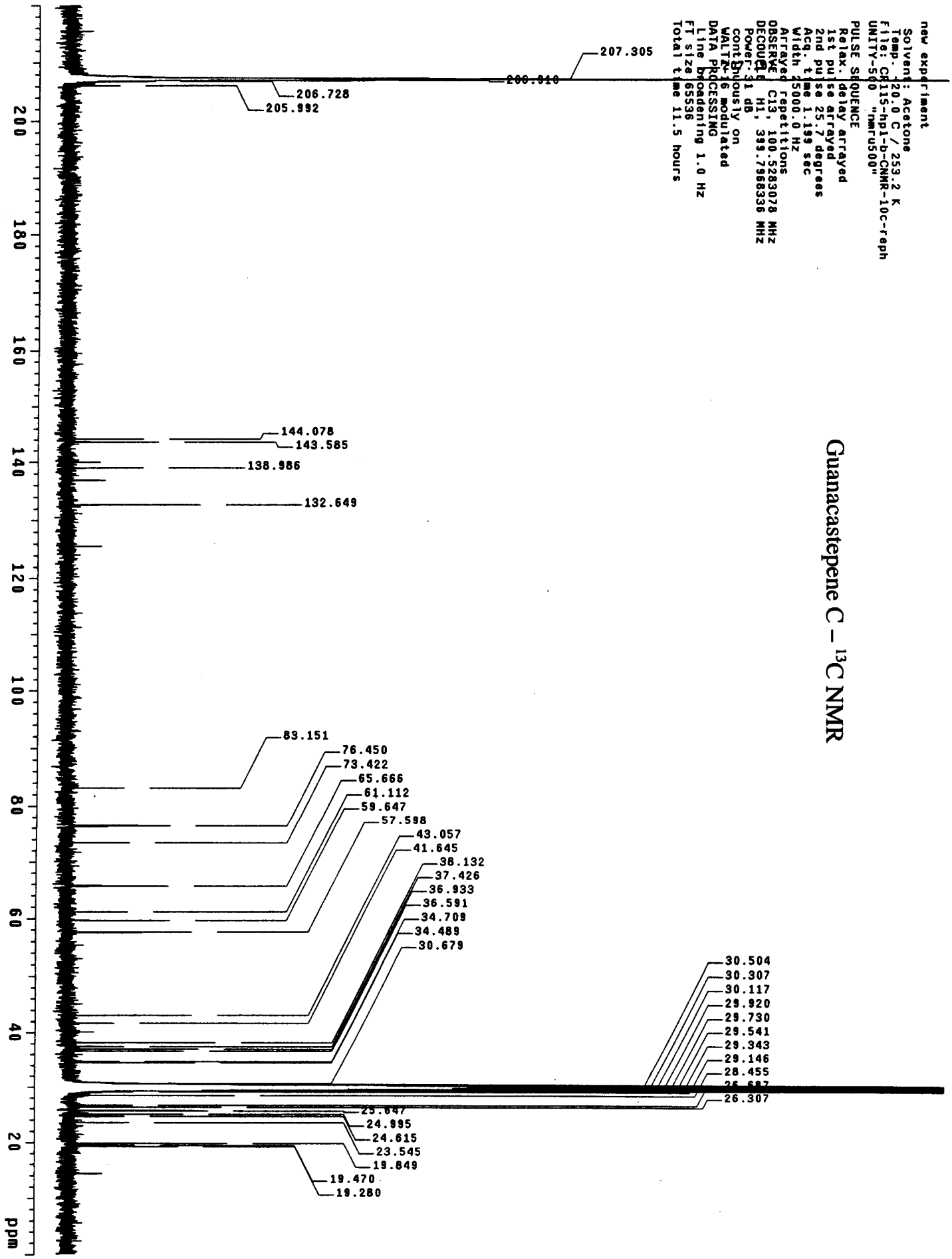
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	18(2)	29(2)	22(2)	0(2)	2(2)	4(2)
O(3)	22(2)	42(3)	36(3)	13(3)	4(2)	11(2)
O(2)	29(2)	31(3)	15(3)	0(2)	-2(2)	1(2)
O(4)	15(2)	35(3)	37(3)	1(2)	7(2)	9(2)
O(6)	26(2)	36(3)	23(3)	-1(2)	5(2)	1(2)
O(5)	35(3)	48(4)	96(4)	1(4)	22(3)	-7(3)
C(1)	19(3)	21(3)	23(4)	-1(3)	4(3)	1(3)
C(2)	27(3)	24(4)	9(3)	7(3)	10(3)	9(3)
C(3)	24(3)	13(4)	13(4)	-2(3)	-1(3)	2(3)
C(4)	20(3)	22(4)	28(4)	1(3)	6(3)	3(3)
C(5)	18(3)	36(5)	32(4)	2(4)	6(3)	1(3)
C(6)	20(4)	44(5)	30(5)	5(4)	0(3)	-1(4)
C(7)	15(3)	23(5)	38(5)	2(4)	0(3)	0(4)
C(8)	22(3)	27(4)	22(4)	-1(3)	5(3)	-3(3)
C(9)	24(3)	32(5)	25(4)	3(3)	6(3)	1(3)
C(10)	21(3)	45(5)	22(5)	-4(4)	3(3)	-4(3)
C(11)	18(3)	26(4)	17(4)	0(3)	2(2)	2(3)
C(12)	23(3)	24(4)	30(4)	3(3)	7(3)	4(3)
C(13)	21(3)	31(4)	29(4)	2(4)	0(3)	8(4)
C(14)	25(3)	9(3)	27(4)	-3(4)	3(3)	7(3)
C(15)	20(3)	17(3)	27(4)	-5(4)	-2(3)	0(3)
C(16)	28(4)	40(5)	32(5)	7(4)	1(4)	-3(4)
C(17)	30(4)	22(4)	24(4)	-5(3)	5(3)	3(3)
C(18)	20(3)	45(5)	19(4)	-5(3)	-6(3)	-5(3)
C(19)	46(5)	64(6)	35(6)	-7(5)	0(4)	-8(4)
C(20)	87(6)	57(5)	41(5)	13(5)	-20(4)	-2(5)
C(21)	16(3)	60(6)	34(4)	4(5)	1(3)	-4(4)
C(22)	24(4)	67(6)	39(5)	-8(5)	4(4)	11(4)

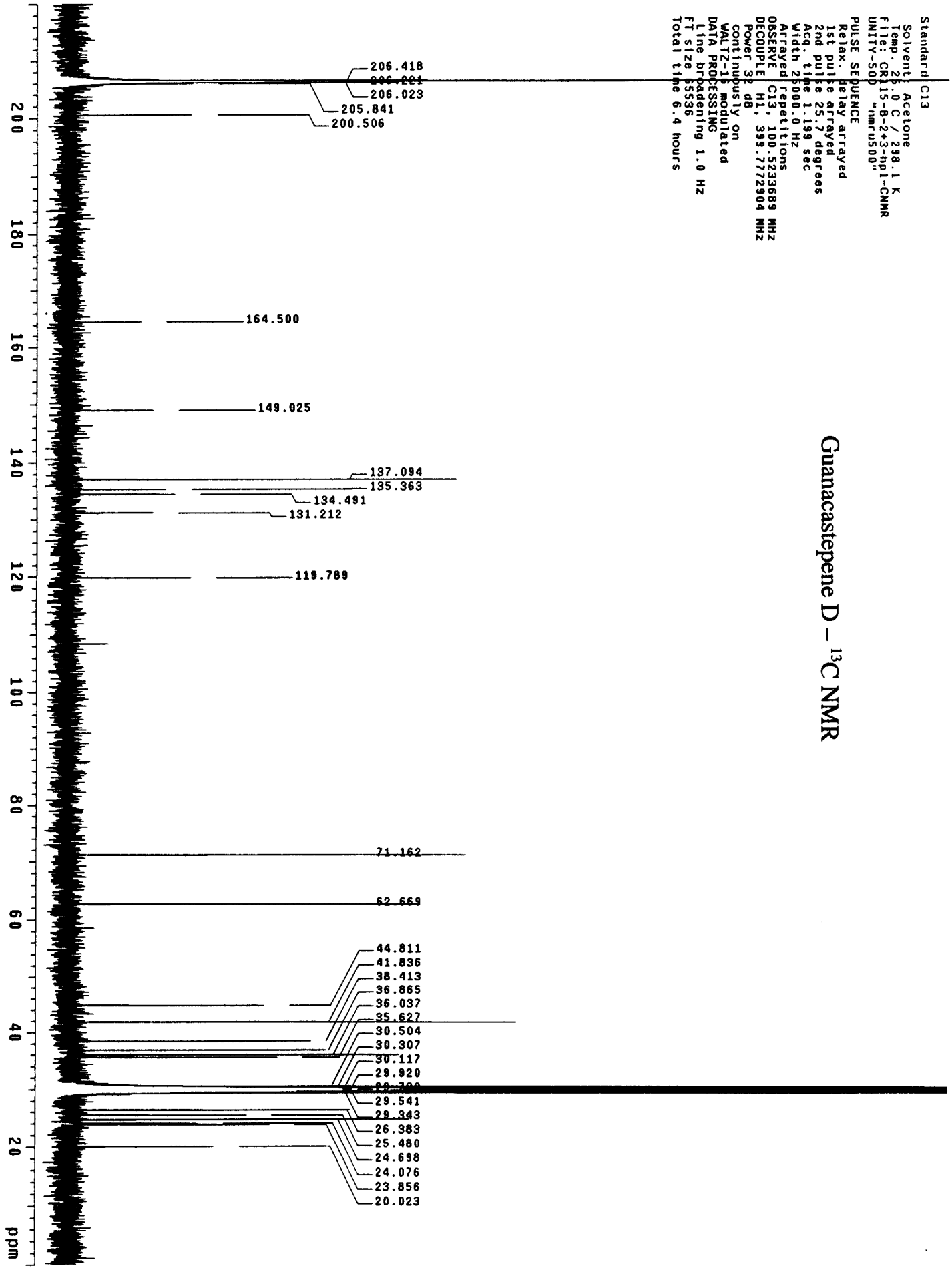
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for guanacastepene O.

	x	y	z	U(eq)
H(20A)	659(11)	7007(19)	499(17)	98
H(20B)	764(7)	6504(12)	-840(30)	98
H(20C)	1255(10)	7910(50)	80(6)	98
H(13)	1105(16)	2180(80)	2190(30)	0(13)
H(19C)	539(15)	3040(70)	460(30)	0(12)
H(12)	1515(15)	6180(80)	1780(40)	2(12)
H(6B)	4250(18)	6660(90)	4300(40)	28(17)
H(16C)	3530(20)	8420(130)	3510(50)	70(20)
H(10B)	2414(17)	6860(80)	1600(40)	15(13)
H(16B)	3374(19)	8470(100)	2190(40)	47(17)
H(7B)	3943(17)	3370(90)	2850(40)	0(16)
H(16A)	2949(17)	8220(80)	3010(30)	1(12)
H(9B)	3091(17)	2900(100)	1640(30)	7(13)
H(17B)	1850(20)	390(110)	1730(50)	48(19)
H(19B)	711(18)	2700(80)	-690(50)	19(16)
H(9)	3298(18)	5340(90)	1160(40)	32(15)
H(5A)	4196(17)	4670(80)	5800(40)	30(15)
H(17B)	2048(19)	1470(90)	620(50)	49(18)
H(6A)	4604(19)	4710(70)	4120(30)	5(13)
H(19A)	1040(40)	1130(180)	260(90)	170(40)
H(17A)	2520(30)	740(130)	1760(60)	110(30)
H(18)	1521(18)	4190(70)	-40(40)	18(13)
H(10A)	2370(20)	4800(90)	710(50)	35(18)
H(7A)	4100(20)	5780(110)	2340(50)	70(20)
H(22C)	-80(20)	6780(120)	2530(50)	70(20)
H(22B)	-70(30)	5500(120)	3710(60)	90(30)
H(22A)	-470(30)	4590(110)	2620(50)	60(20)
H(3O)	4030(40)	1050(160)	5330(80)	160(50)

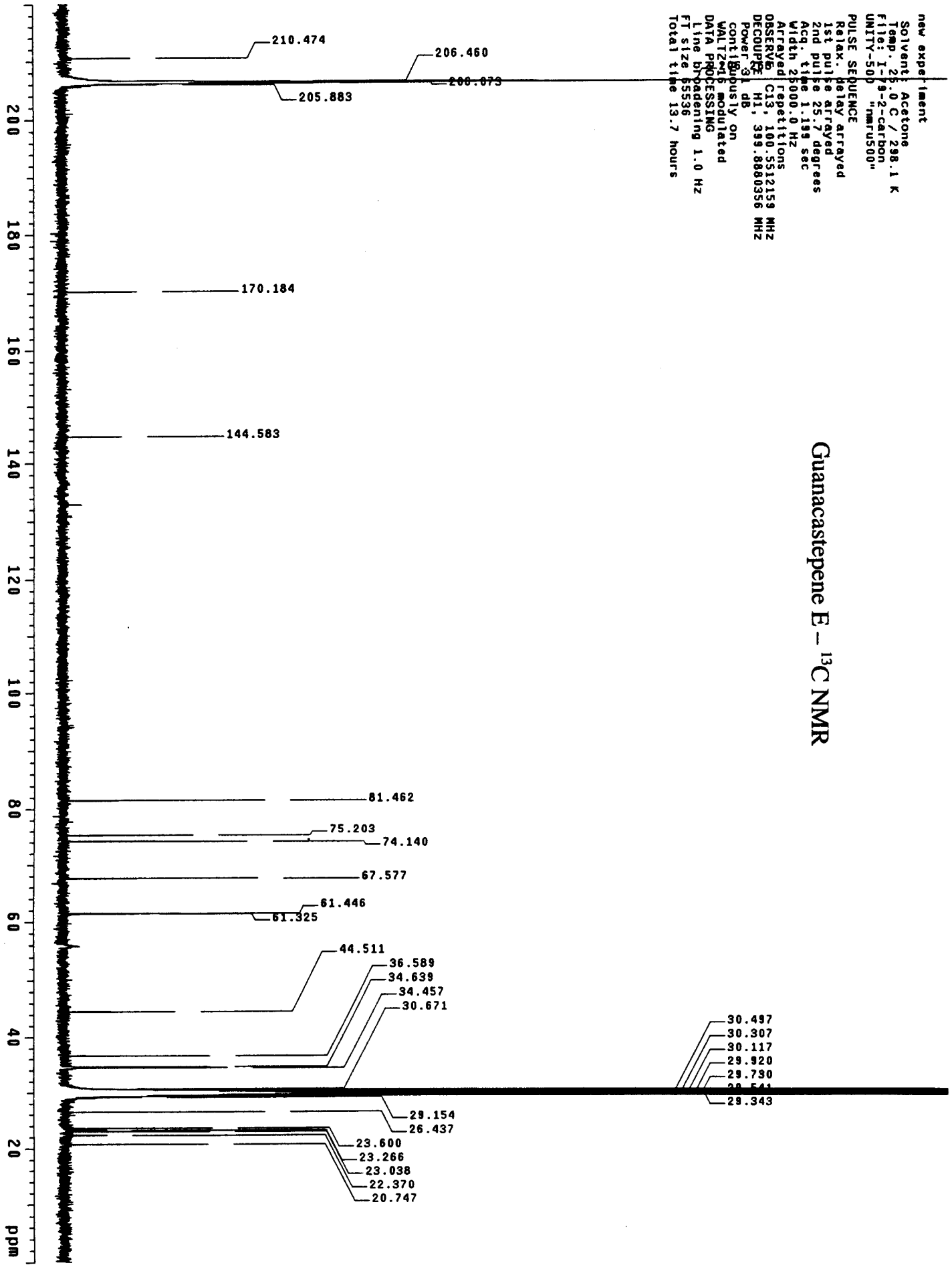


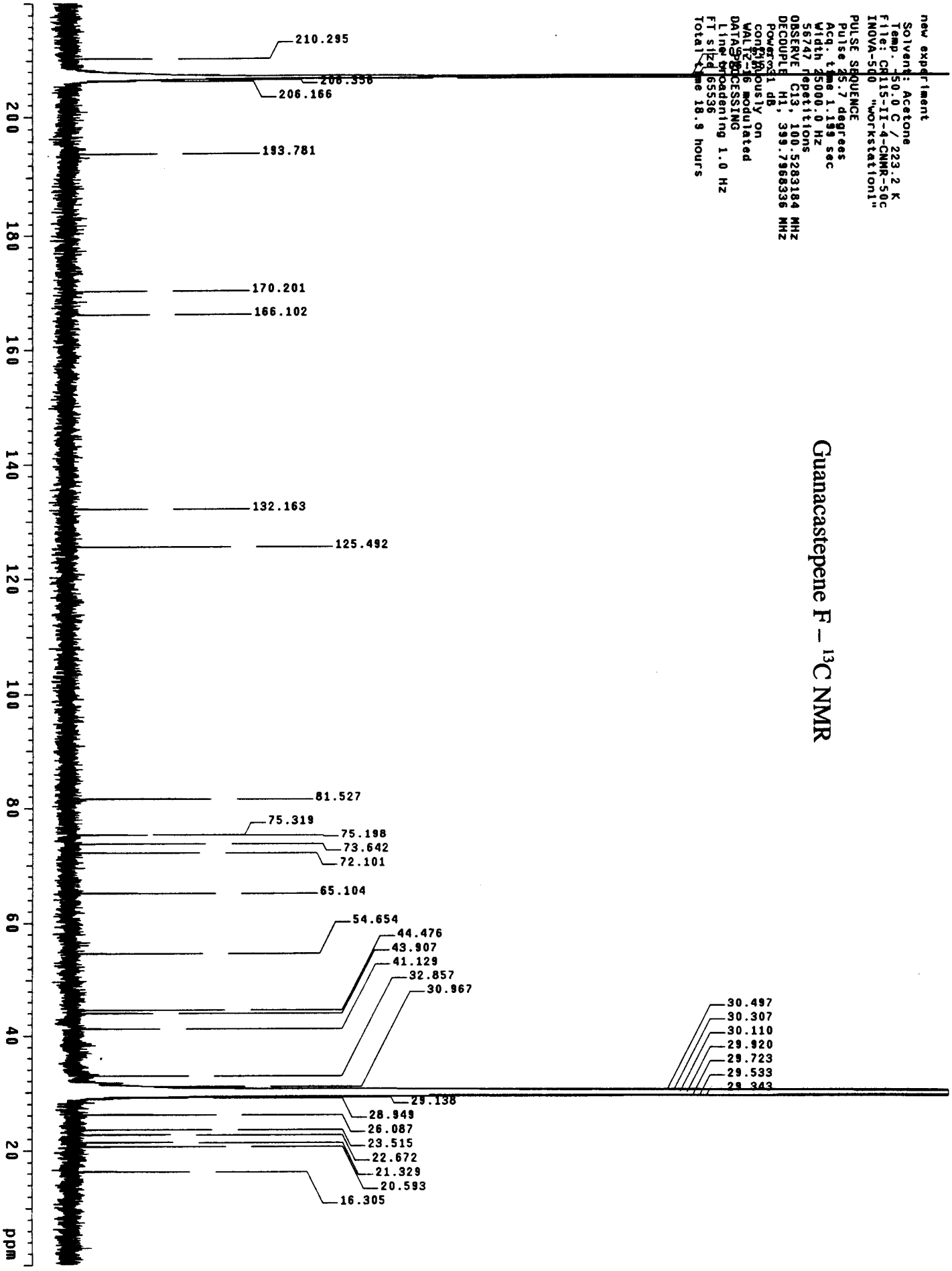
Guanacastepene B – ^{13}C NMR

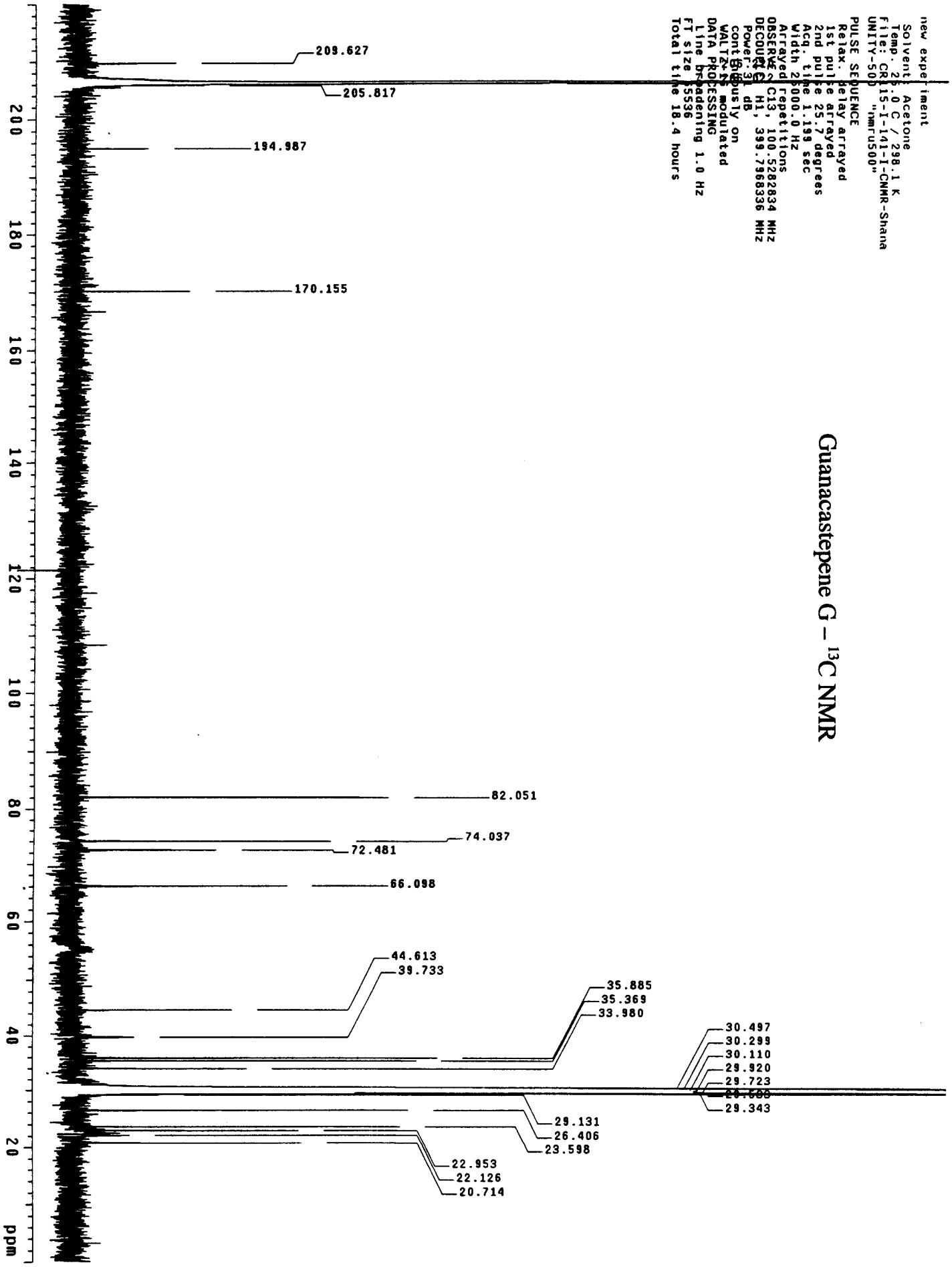

new experiment
Solvent: Acetone
Temp. -20.0 C / 253.2 K
File: CR115-hp1-b-CNMR-10c-reph
UNITY-500 "nmru500"
PULSE SEQUENCE
Relax. delay arrayed
1st pulse arrayed
2nd pulse 25.7 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
Arrayed repetitions
OBSERVE C13, 100.5283078 MHz
DECOUPLE H1, 399.7966336 MHz
Power 31 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 11.5 hours
207.305
206.910
206.728
205.992
144.078
143.585
138.986
132.649
83.151
76.450
73.422
65.666
61.112
59.647
57.598
43.057
41.645
38.132
37.426
36.933
36.591
34.709
34.489
30.679
30.504
30.307
30.117
29.920
29.730
29.541
29.343
29.146
28.455
26.307
25.647
24.995
24.615
23.545
19.849
19.470
19.280
200
180
160
140
120
100
80
60
40
20
ppm
Guanacastepene C – ^{13}C NMR



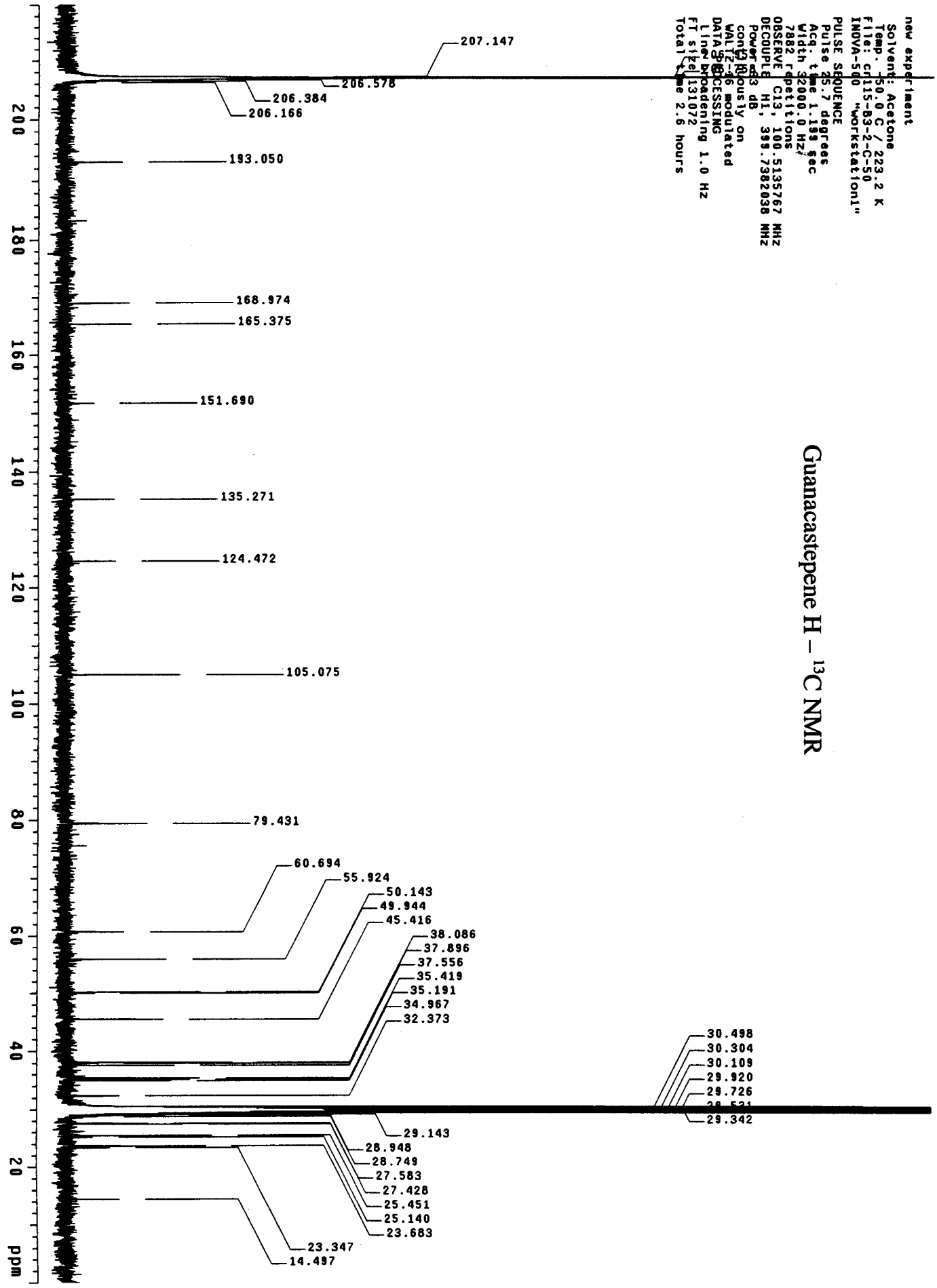
Guanacastepene D – ^{13}C NMR


new experiment
Solvent: Acetone
Temp. 25.0 C / 298.1 K
File: I-79-2-carbon
UNITY-500 "nmru500"
PULSE SEQUENCE
Relax. delay arrayed
1st pulse arrayed
2nd pulse 25.7 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
Arrayed repetitions
OBSERVE C13, 100.5512159 MHz
DECOUPLE H1, 399.8880356 MHz
Power 31 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 13.7 hours
Guanacastepene E – ^{13}C NMR
210.474
206.460
205.883
170.184
144.583
81.462
75.203
74.140
67.577
61.446
61.325
44.511
36.589
34.639
34.457
30.671
30.497
30.307
30.117
29.920
29.730
29.343
29.154
26.437
23.600
23.266
23.038
22.370
20.747
200
180
160
140
120
100
80
60
40
20
ppm

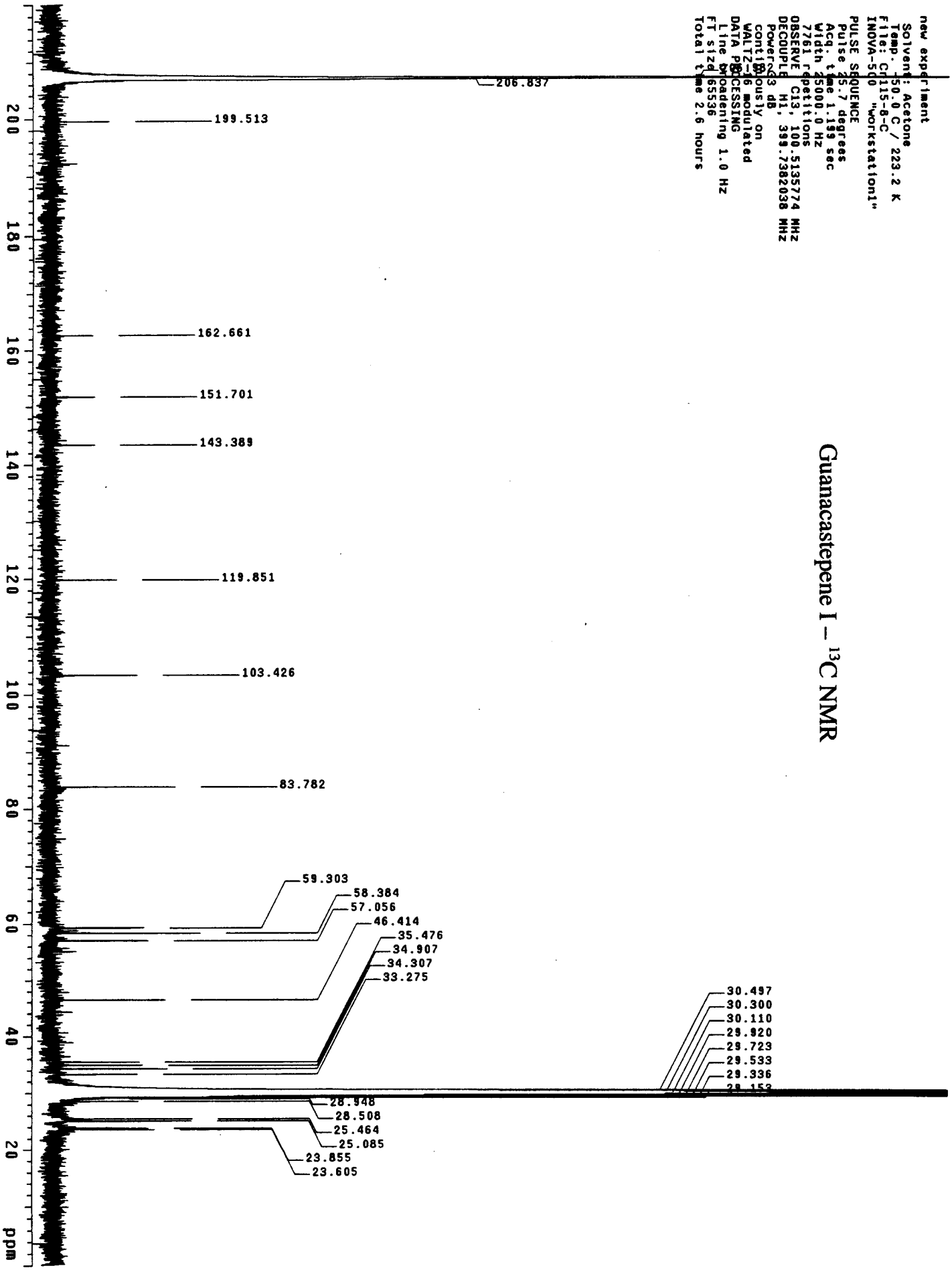

new experiment
Solvent: Acetone
Temp. 50.0 C / 223.2 K
File: CR115-II-4-CNMR-50c
INOVA-500 "workstation1"
PULSE SEQUENCE
Pulse 25.7 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
56747 repetitions
OBSERVE C13, 100.5283184 MHz
DECOUPLE H1, 399.7968336 MHz
Power 51 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 18.9 hours
Guanacastepene F – 13C NMR
210.295
206.356
206.166
193.781
170.201
166.102
132.163
125.492
81.527
75.319
75.198
73.642
72.101
65.104
54.654
44.476
43.907
41.129
32.857
30.967
30.497
30.307
30.110
29.920
29.723
29.533
29.343
29.138
28.949
26.087
23.515
22.672
21.329
20.593
16.305
200
180
160
140
120
100
80
60
40
20
ppm



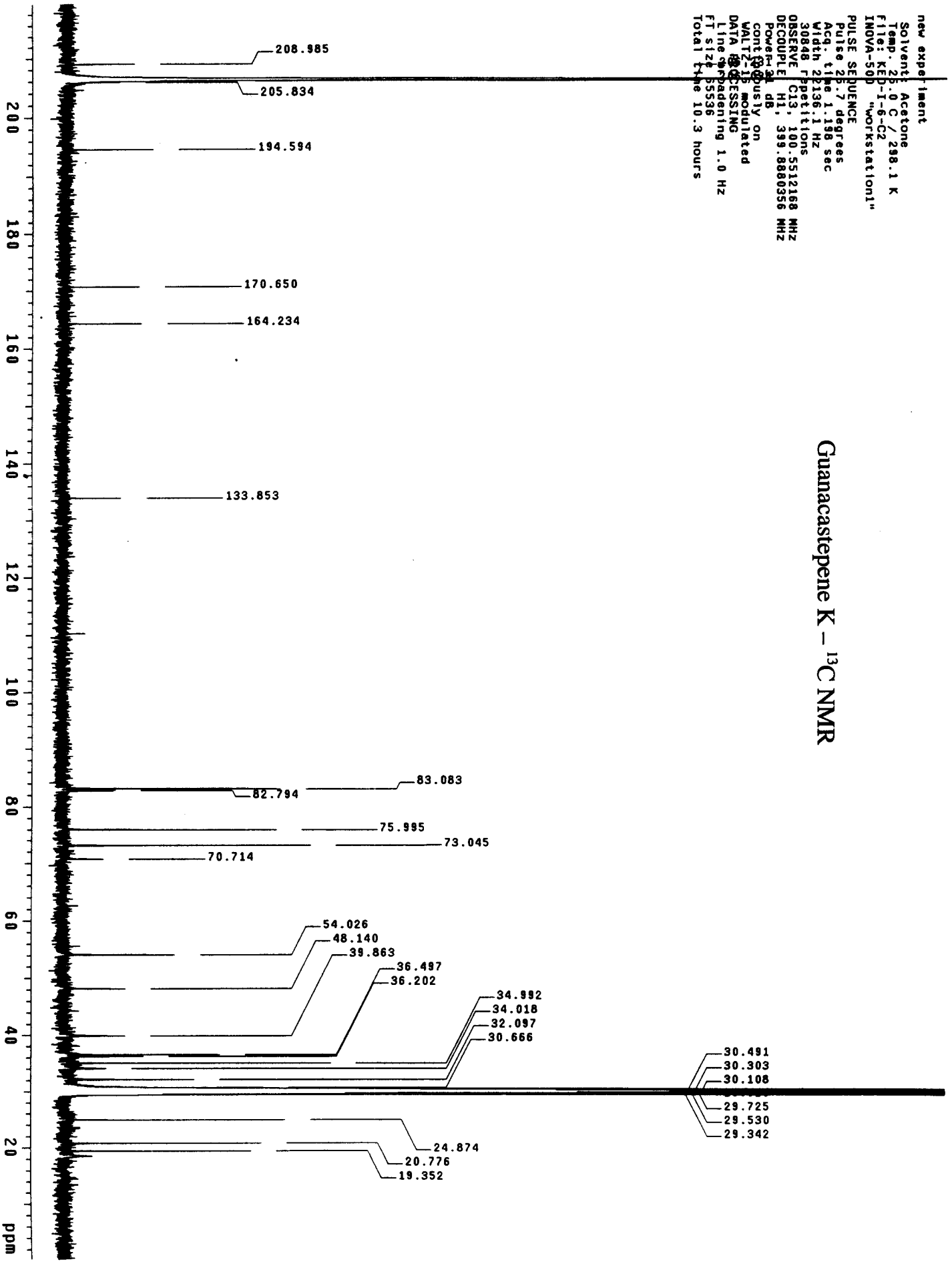
Guanacastepene G – ^{13}C NMR



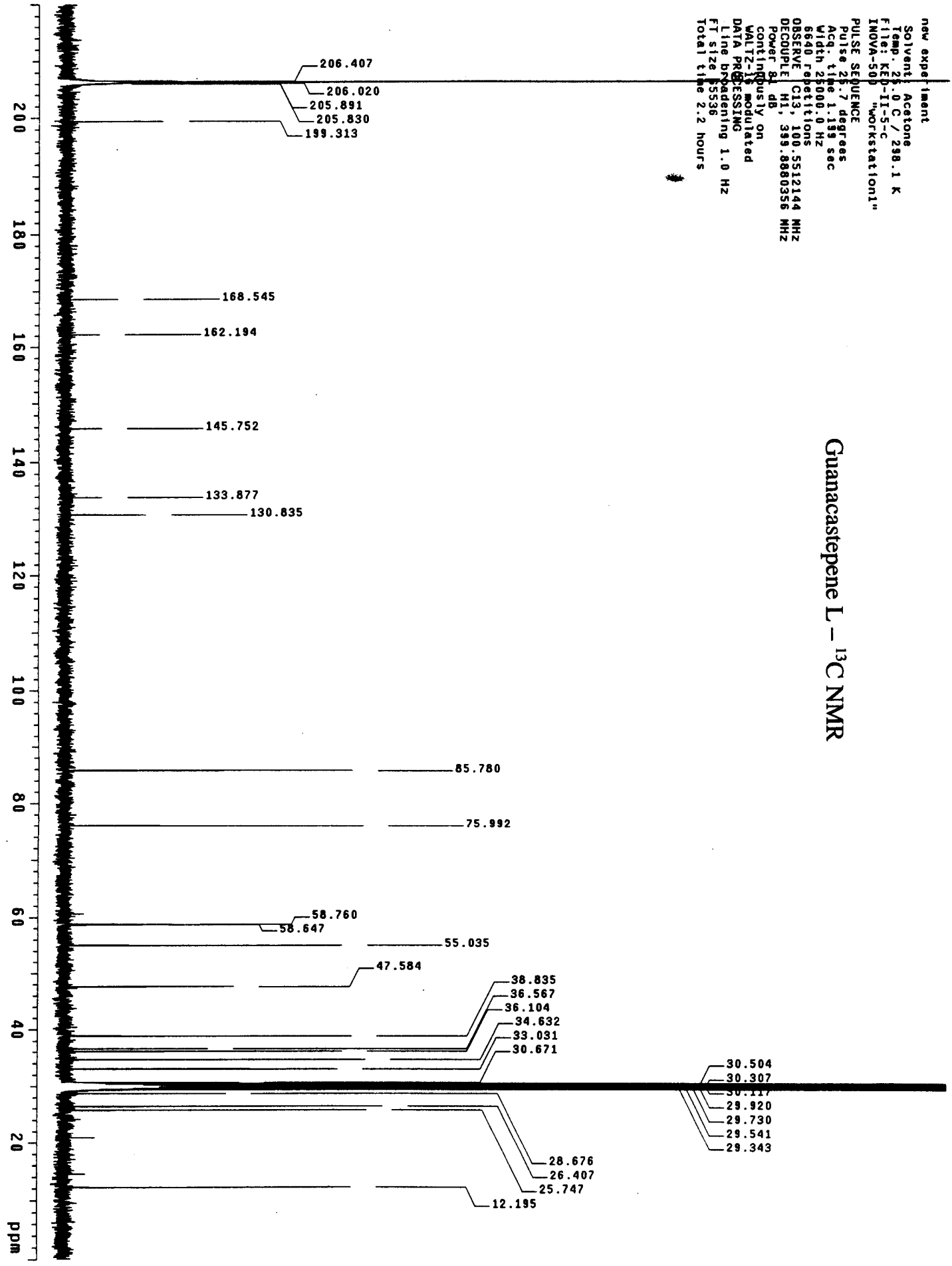
Guanacastepene H – ^{13}C NMR



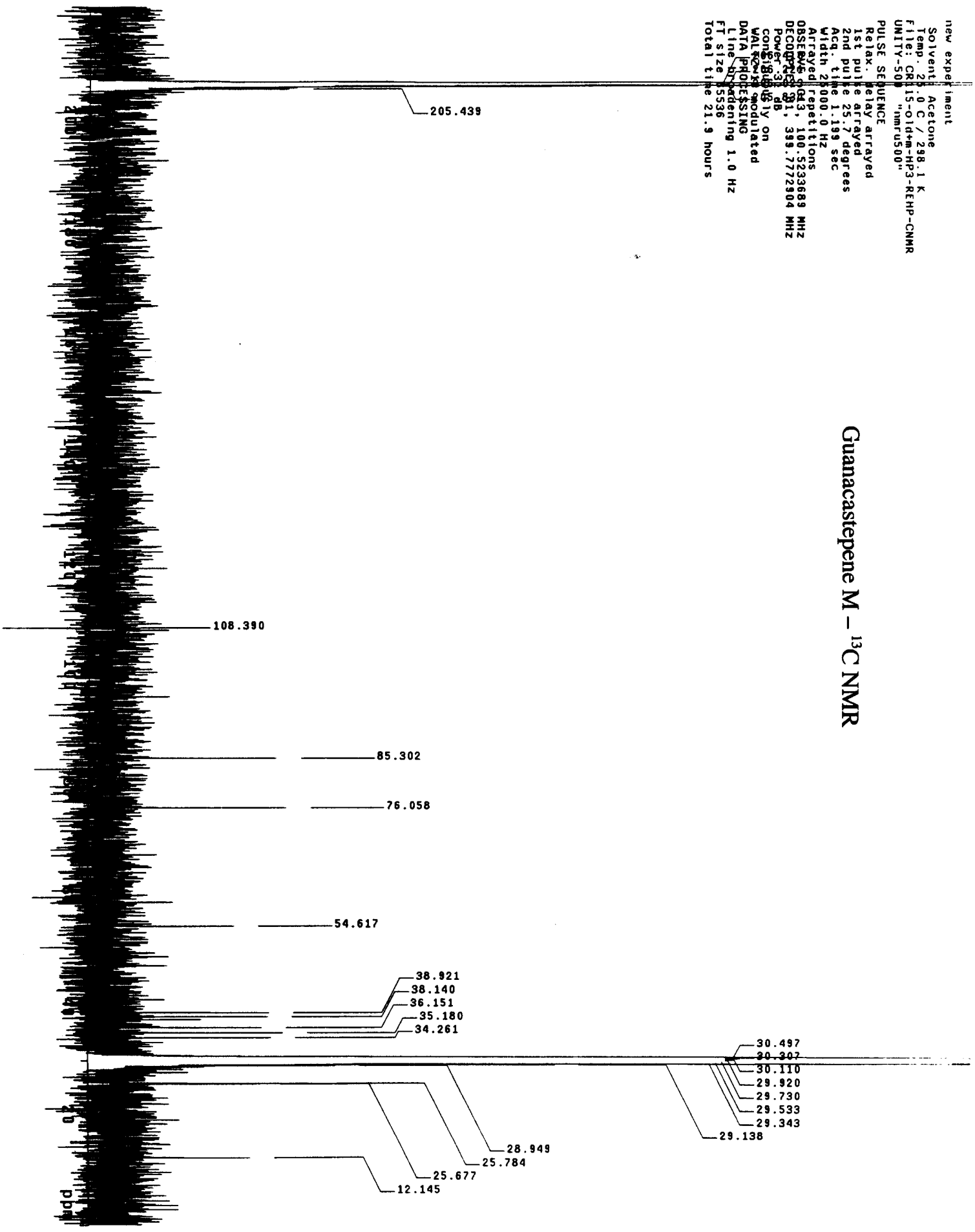
Guanacastepene I – ^{13}C NMR



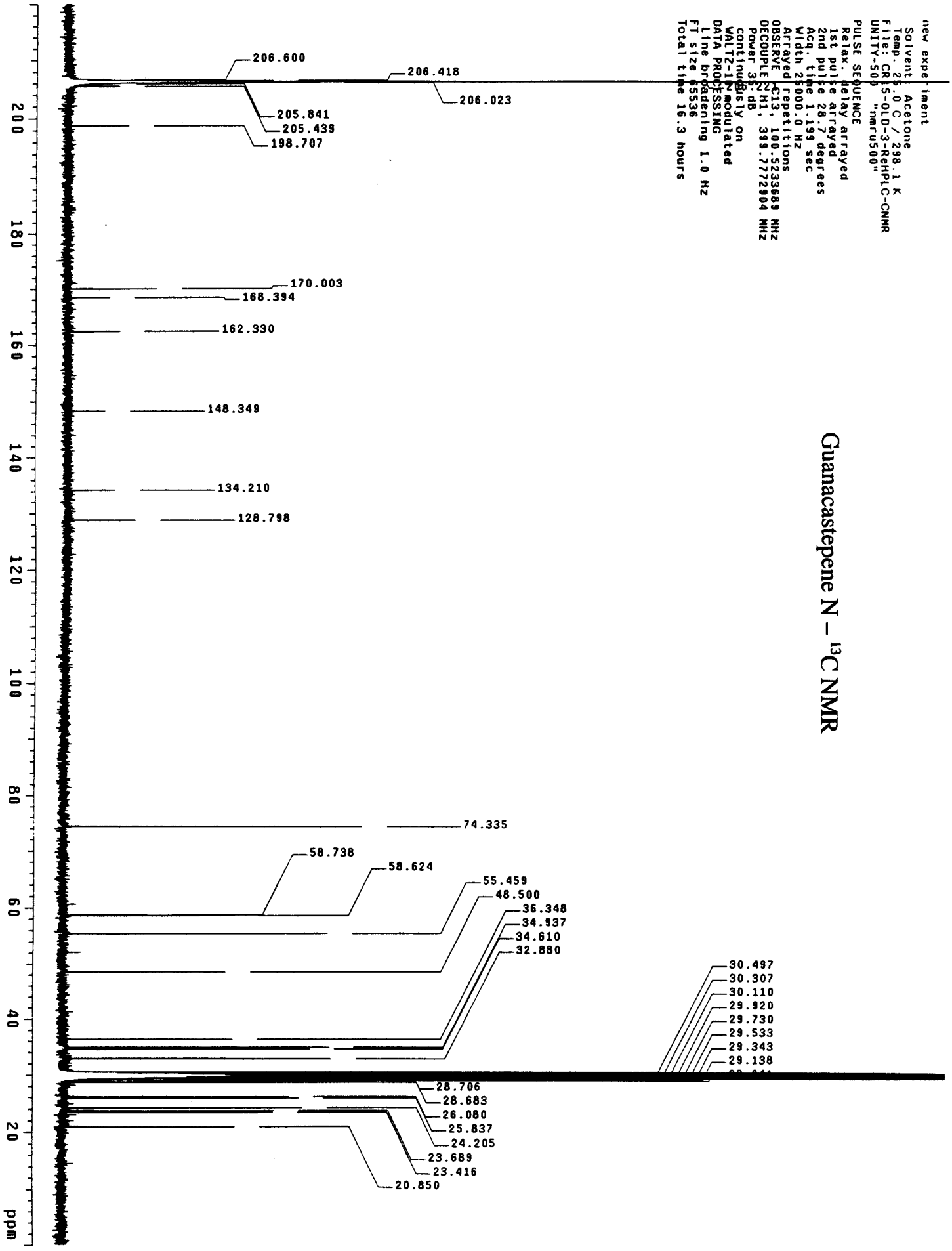
Guanacastepene K – ^{13}C NMR



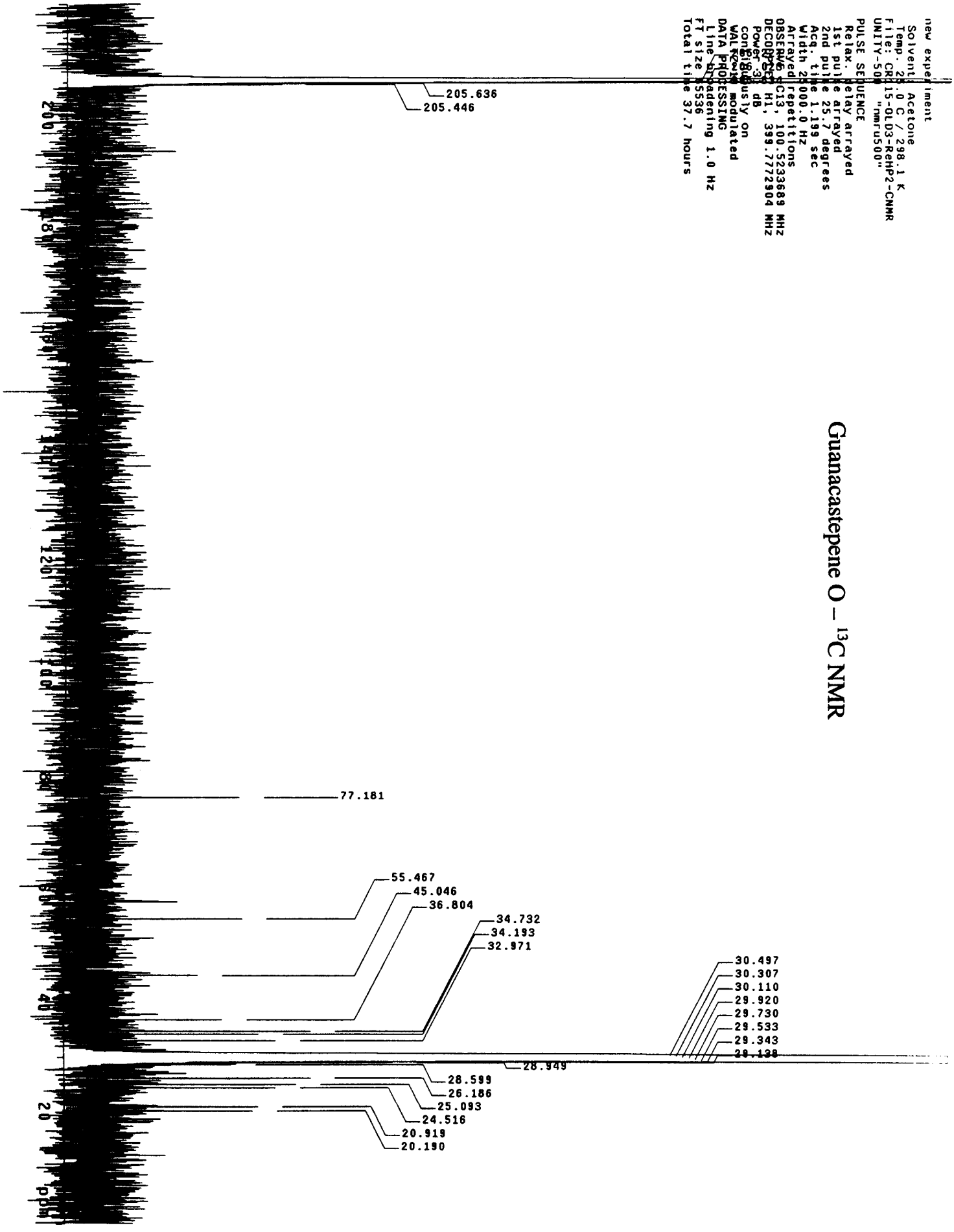
Guanacastepene L – ^{13}C NMR



Guanacastepene M – ^{13}C NMR



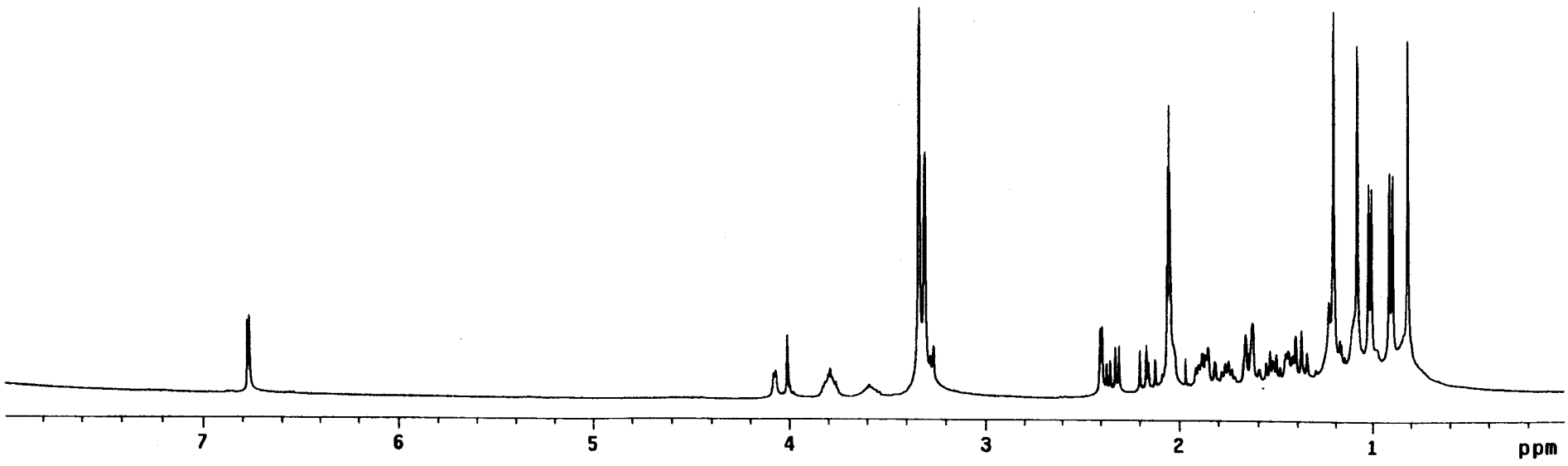
Guanacastepene N – ^{13}C NMR



Guanacastepene O – ^{13}C NMR

Guanacastepene B – ^{1}H NMR

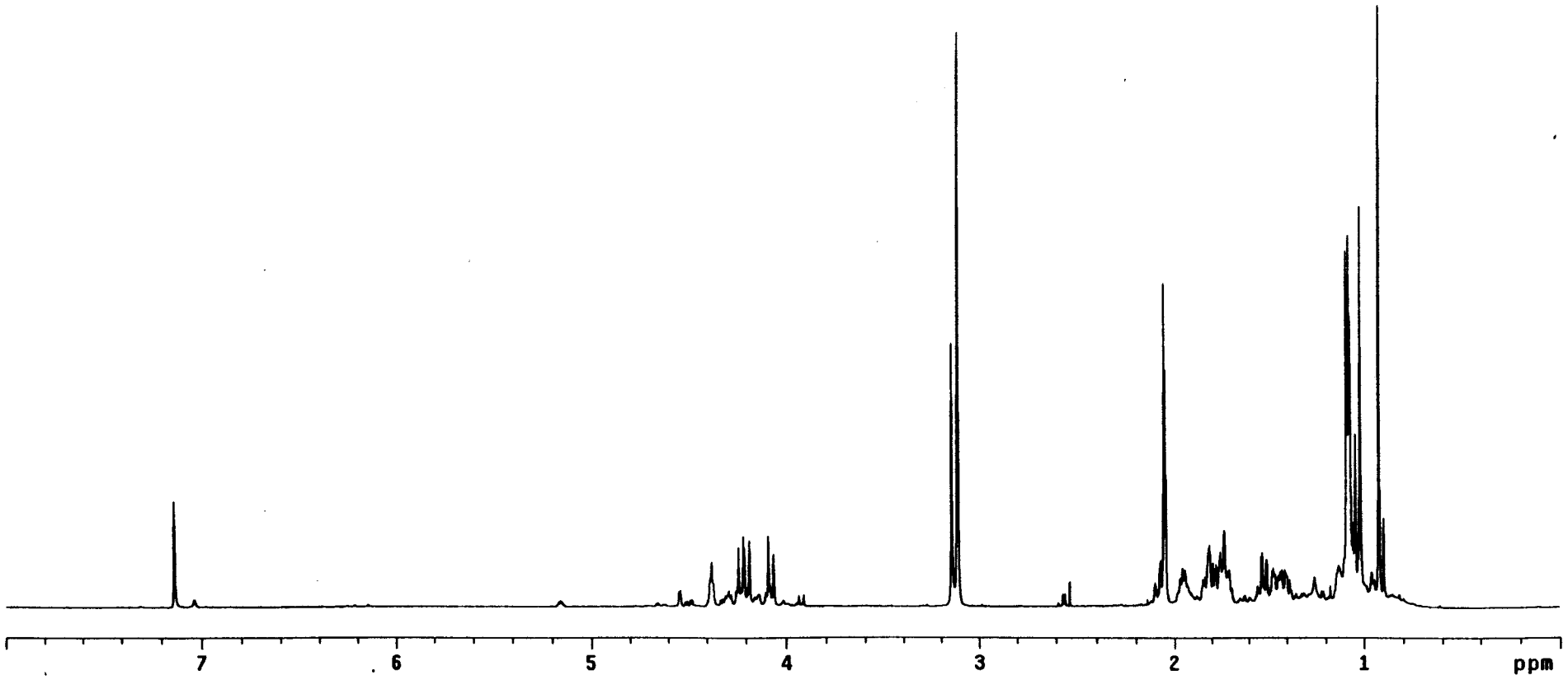
```
STANDARD 1H OBSERVE

 Solvent: Acetone
 Temp. -50.0 C / 223.2 K
File: CR115-HPII-D-HNMR-50C-400
INOVA-500  "workstation1"
PULSE SEQUENCE
 Pulse 58.7 degrees
 Acq. time 2.003 sec
 Width 3195.7 Hz
 160 repetitions
OBSERVE   H1, 399.7944110 MHz
DATA PROCESSING
 Line broadening 0.1 Hz
FT size 16384
Total time 5 minutes
```



STANDARD PROTON PARAMETERS
Solvent: Acetone
Temp. -10.0 C / 263.1 K
File: CR115-hp1-b-HNMR-10C
UNITY-500 "nmru500"

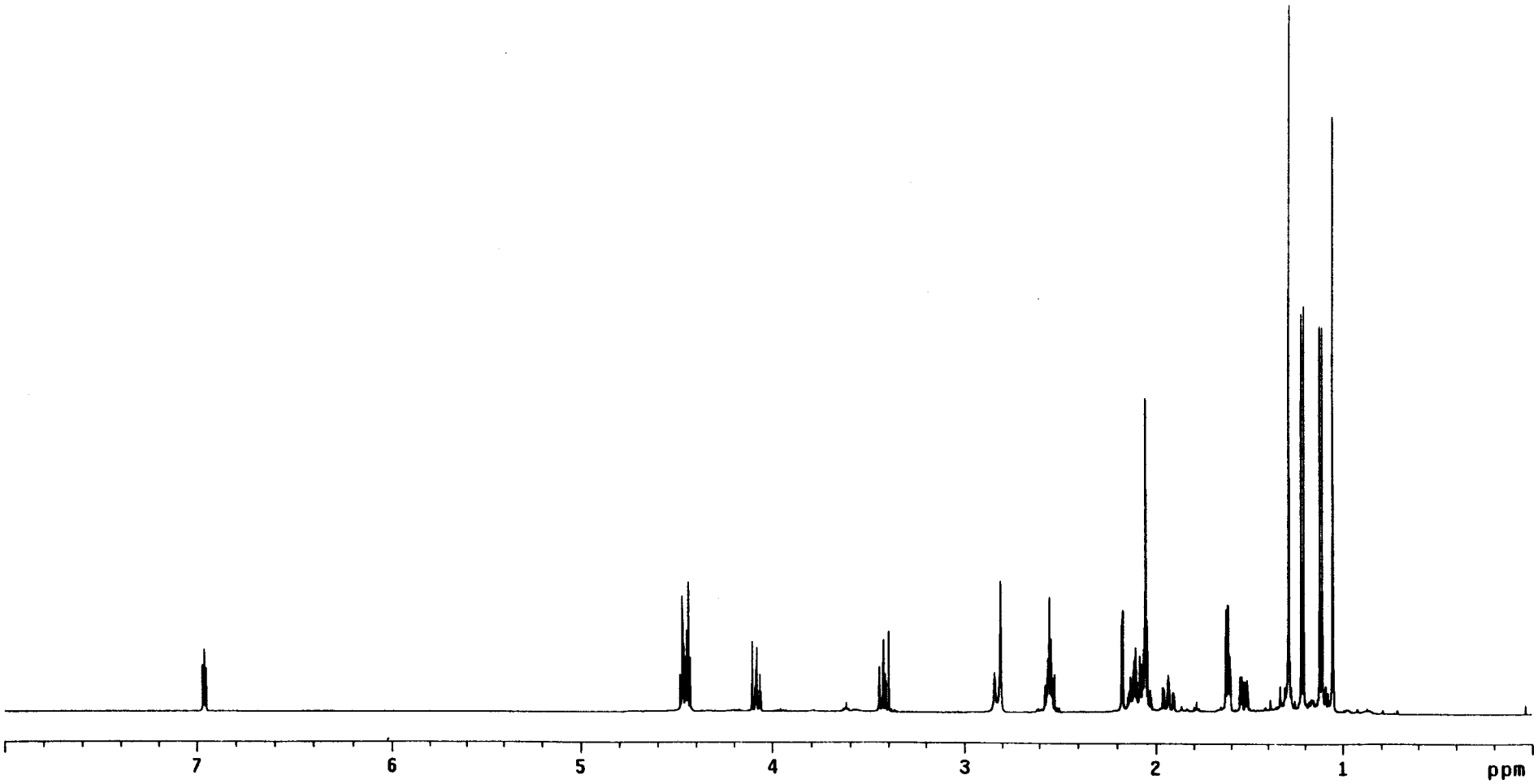
PULSE SEQUENCE
Relax. delay arrayed
1st pulse arrayed
2nd pulse 51.1 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
Arrayed repetitions
OBSERVE H1, 499.9270431 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 8 minutes

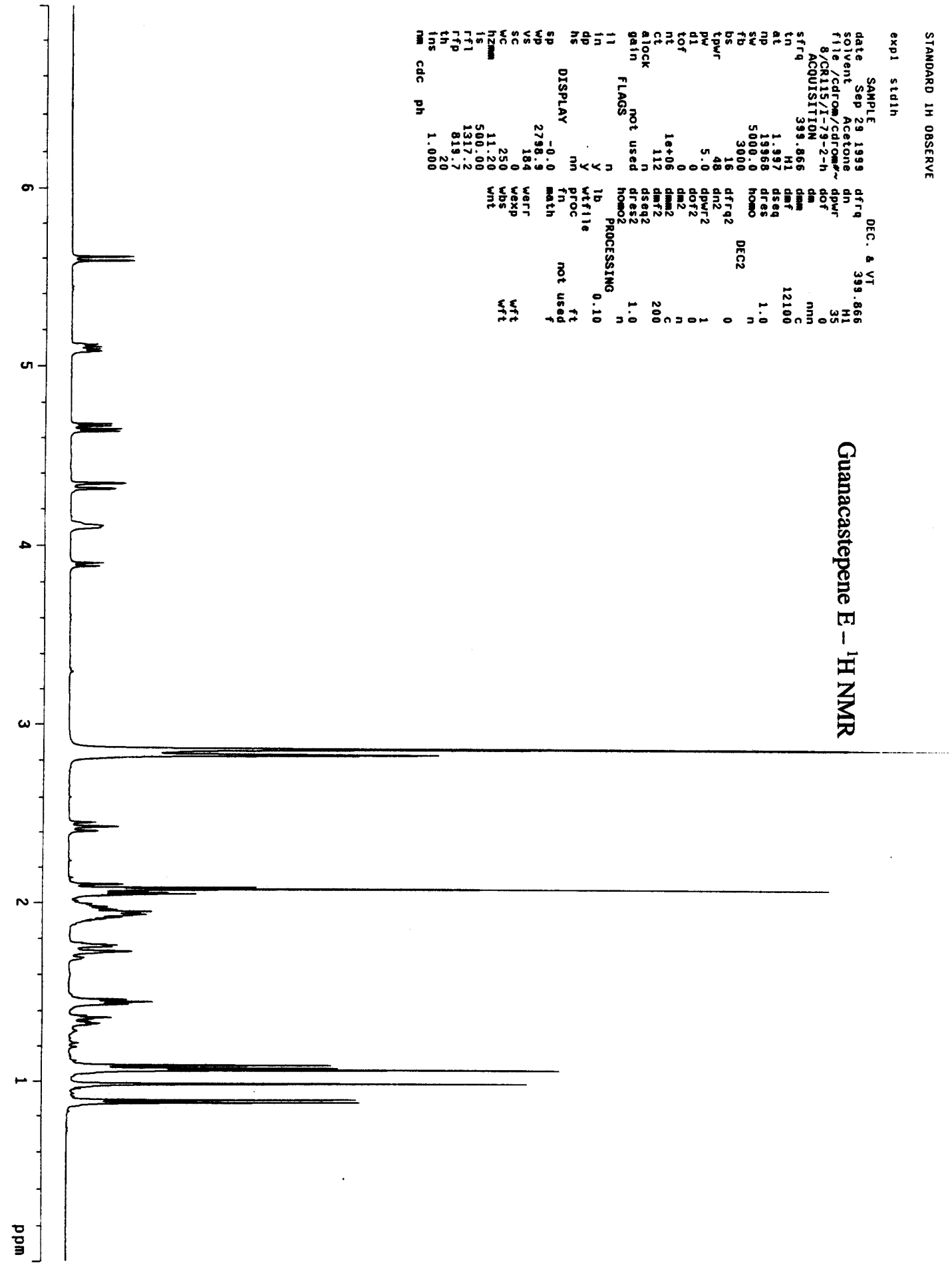
Guanacastepene C – ^{1}H NMR



STANDARD PROTON PARAMETERS
Solvent: Acetone
Temp. 25.0 C / 298.1 K
File: CR115-B-2+3-HP1-HNMR
UNITY-500 "nmru500"
PULSE SEQUENCE
Relax. delay arrayed
1st pulse arrayed
2nd pulse 51.1 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
Arrayed repetitions
OBSERVE H1, 499.9270441 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 24 minutes

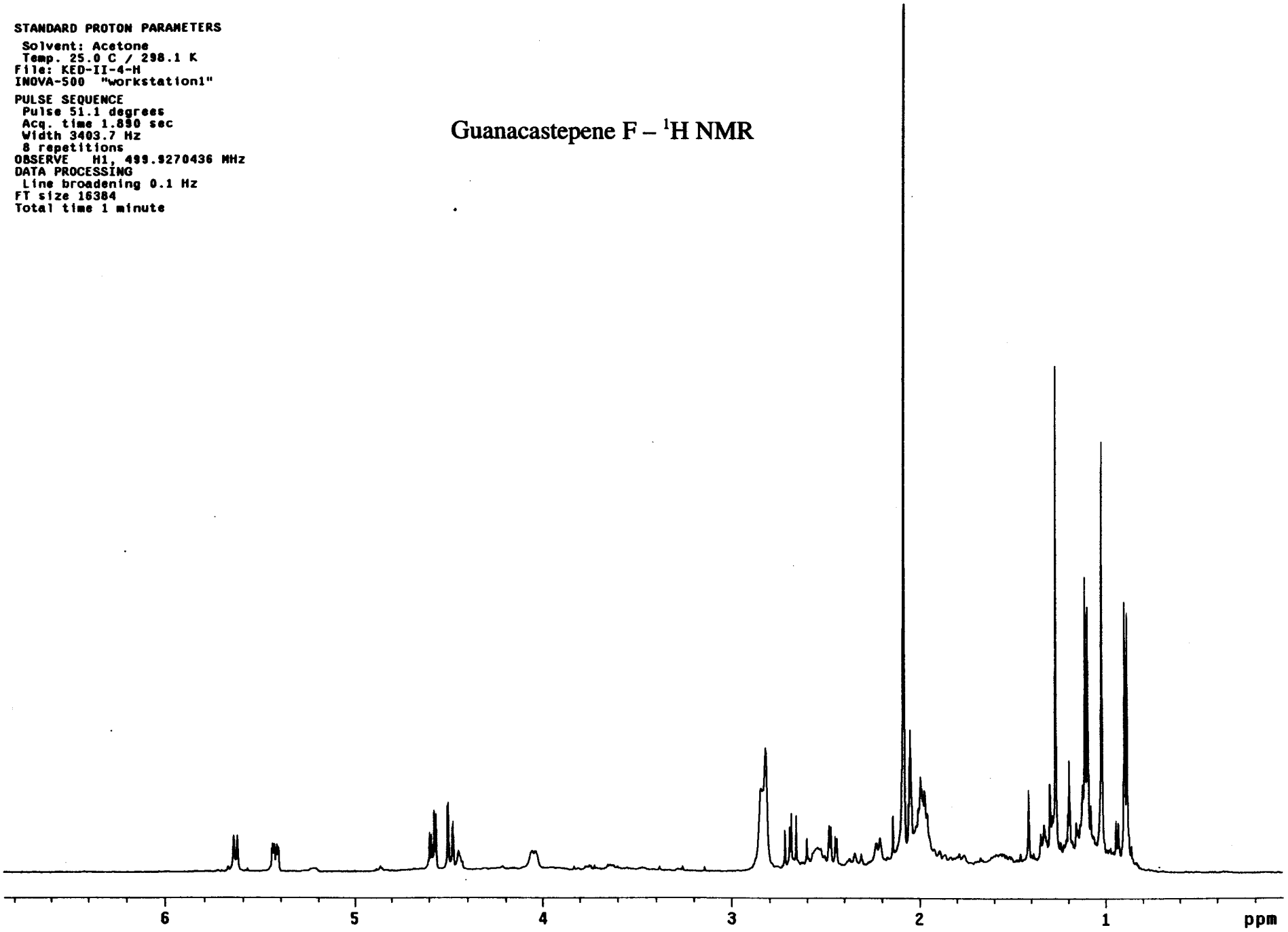
Guanacastepene D – ^{1}H NMR




STANDARD 1H OBSERVE
expl stdih
SAMPLE
date Sep 29 1999
solvent Acetone
file /cdrom/cdrom#~
8/CR115/I-79-2-h
ACQUISITION
sfrq 399.866
tn H1
at 1.997
np 19968
sw 5000.0
fb 3000
bs 16
tpwr 48
pw 5.0
d1 0
tof 0
nt 1e+06
ct 112
alock n
gain not used
FLAGS
il n
in y
dp y
hs nn
DISPLAY
sp -0.0
wp 2798.9
vs 184
sc 0
wc 250
hzmm 11.20
is 500.00
rfl 1317.2
rfp 819.7
th 20
ins 1.000
nm cdc ph
dfrq DEC. & VT
dn 399.866
dpwr H1
dof 35
dm 0
dmm nnn
dmf c
12100
dseq
dres
homo 1.0
DEC2 n
dfrq2
dn2 0
dpwr2
dof2 1
dm2 0
dmm2 n
dmf2 c
dseq2 200
dres2
homo2 1.0
PROCESSING n
lb
wtfile 0.10
proc
fn ft
not used
math not used
werr f
wexp
wbs wft
wnt wft
Guanacastepene E – ^{1}H NMR
6
5
4
3
2
1
ppm

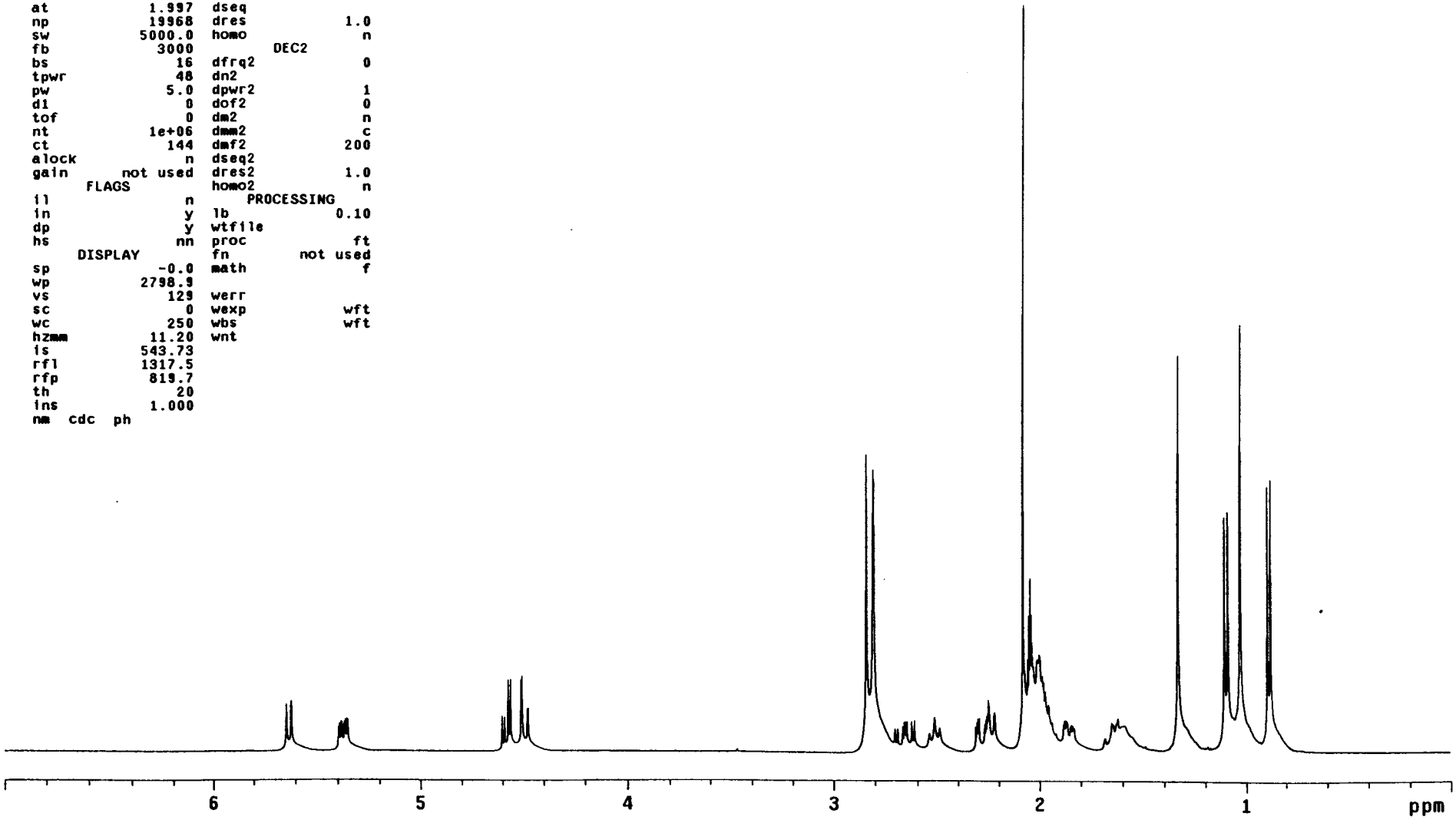
STANDARD PROTON PARAMETERS
Solvent: Acetone
Temp. 25.0 C / 298.1 K
File: KED-II-4-H
INOVA-500 "workstation1"
PULSE SEQUENCE
Pulse 51.1 degrees
Acq. time 1.880 sec
Width 3403.7 Hz
8 repetitions
OBSERVE H1, 499.9270436 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 16384
Total time 1 minute

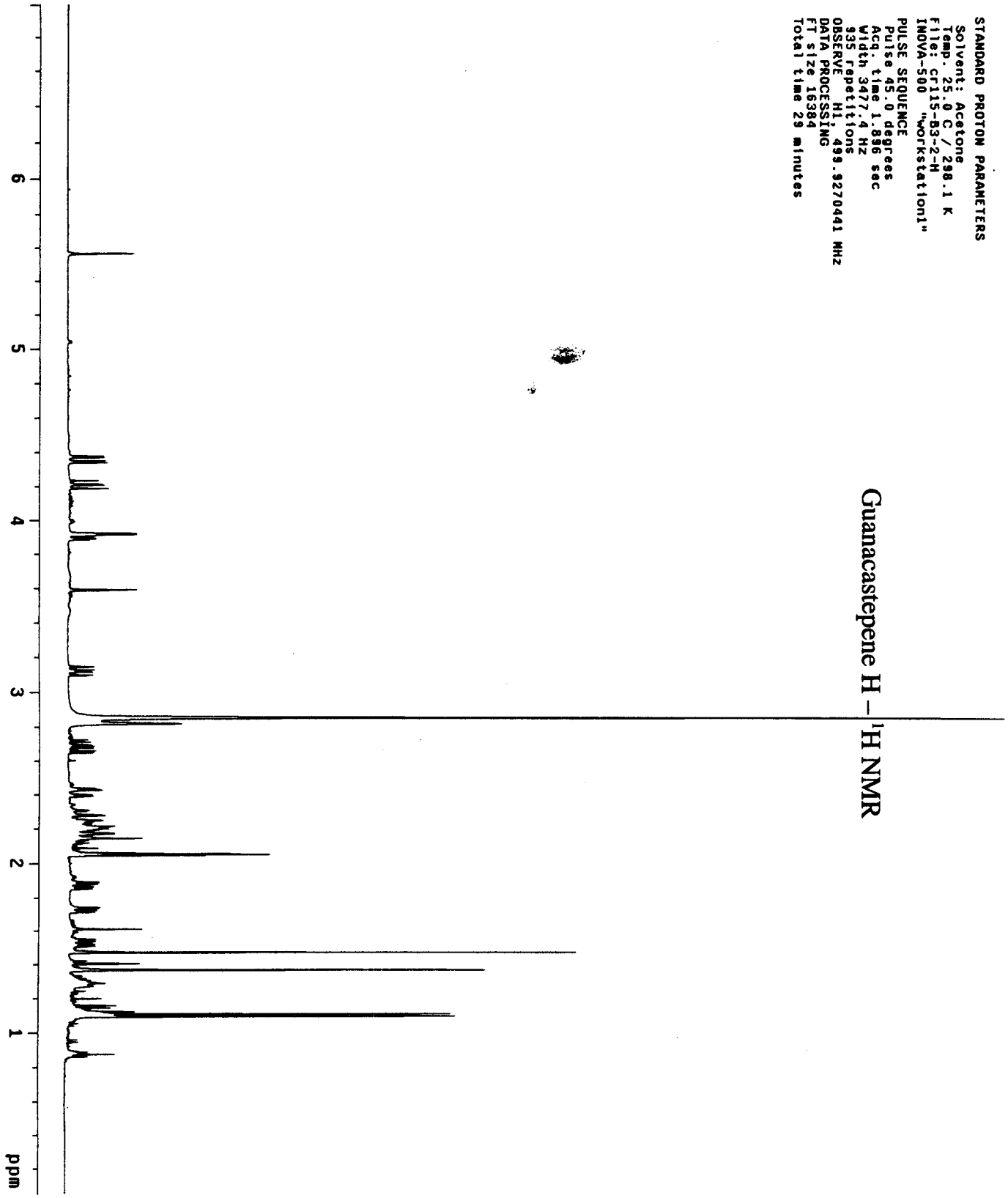
Guanacastepene F – ^{1}H NMR



Guanacastepene G – ^{1}H NMR

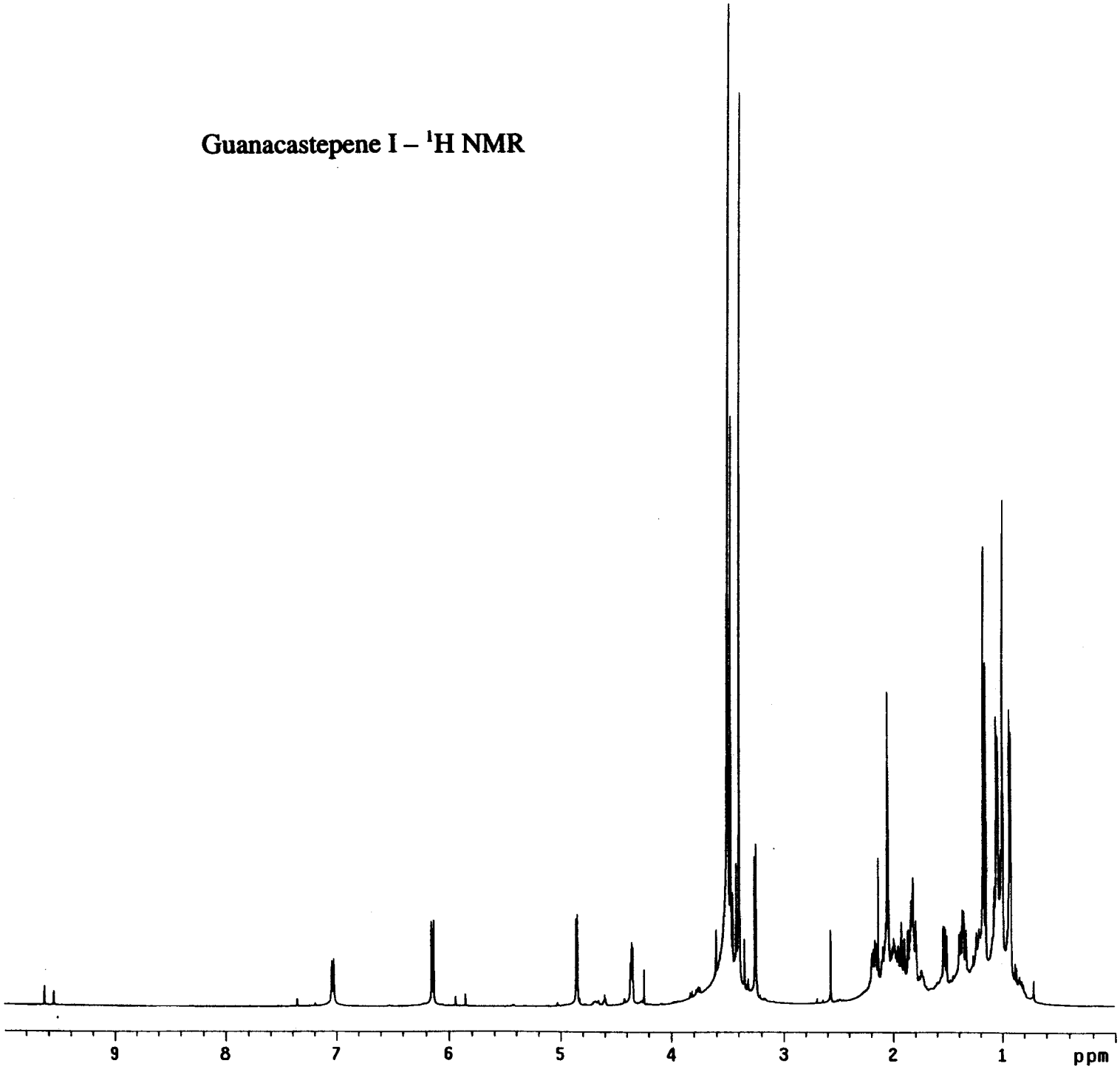
```
STANDARD 1H OBSERVE

exp1  std1h

      SAMPLE
date    Aug 24 1999
solvent     Acetone
file /cdrom/cdrom#~
    8/CR115/I-47-9
   ACQUISITION
sfrq        399.866
tn               H1
at             1.997
np             19968
sw            5000.0
fb              3000
bs                16
tpwr              48
pw               5.0
d1                 0
tof                0
nt             1e+06
ct               144
alock              n
gain       not used
      FLAGS
il                 n
in                 y
dp                 y
hs                nn
     DISPLAY
sp              -0.0
wp            2798.9
vs              129
sc                 0
wc               250
hzmm           11.20
is            543.73
rfl           1317.5
rfp            819.7
th                20
ins            1.000
nm  cdc  ph

      DEC. & VT
dfrq        399.866
dn               H1
dpwr             35
dof               0
dm              nnn
dmm               c
dmf           12100
dseq
dres            1.0
homo              n
      DEC2
dfrq2             0
dn2
dpwr2             1
dof2              0
dm2               n
dmm2              c
dmf2            200
dseq2
dres2           1.0
homo2             n
     PROCESSING
lb             0.10
wtfile
proc              ft
fn         not used
math              f
werr
wexp            wft
wbs             wft
wnt
```

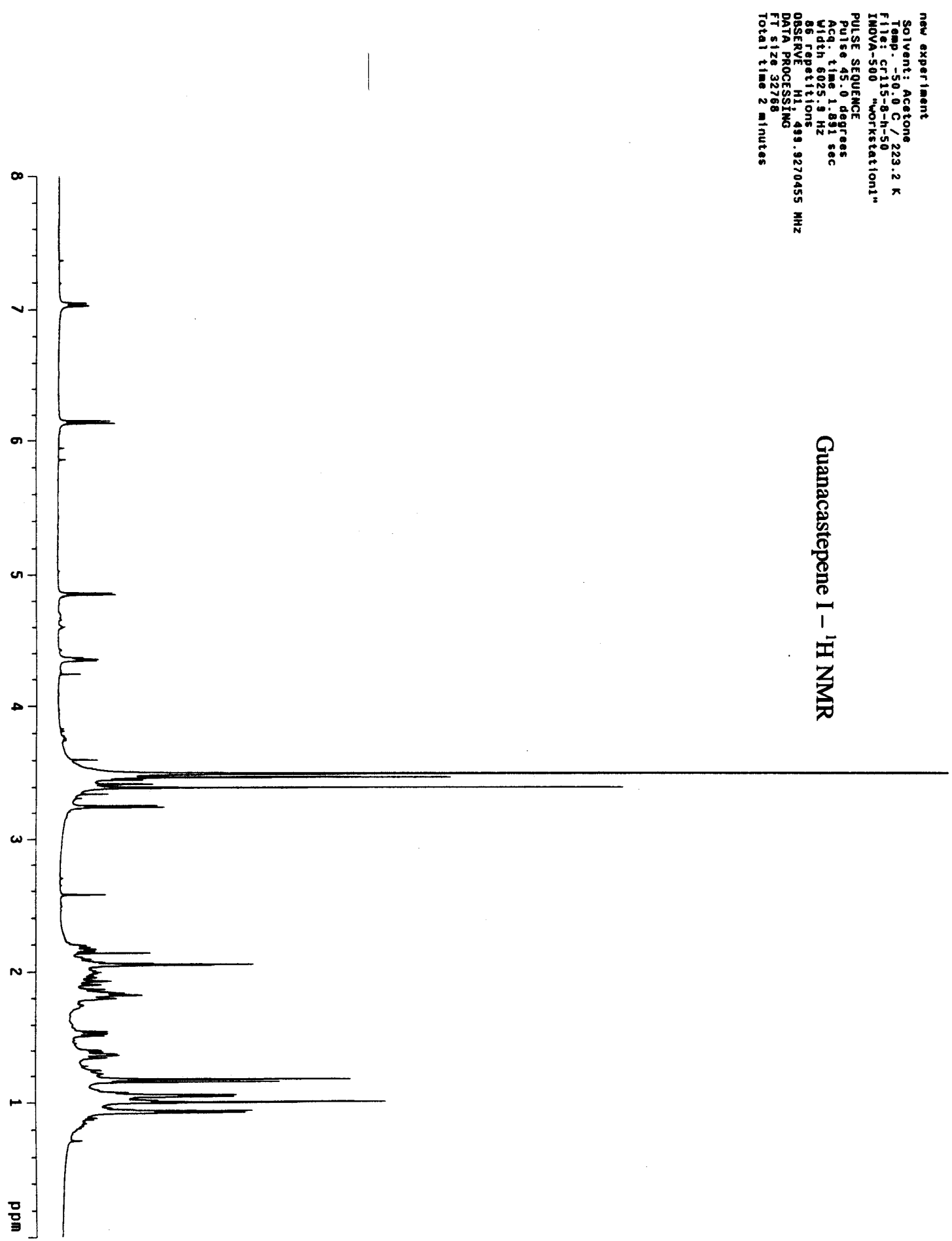



STANDARD PROTON PARAMETERS
Solvent: Acetone
Temp. 25.0 C / 298.1 K
File: cr115-B3-2-H
INOVA-500 "workstation1"
PULSE SEQUENCE
Pulse 45.0 degrees
Acq. time 1.896 sec
Width 3477.4 Hz
935 repetitions
OBSERVE H1, 499.9270441 MHz
DATA PROCESSING
FT size 16384
Total time 29 minutes
Guanacastepene H – ^{1}H NMR
6
5
4
3
2
1
ppm

```
new experiment
 Solvent: Acetone
 Temp. -50.0 C / 223.2 K
File: cr115-8-h-50
UNITY-500  "nmru500"
PULSE SEQUENCE
 Relax. delay arrayed
 1st pulse arrayed
 2nd pulse 45.0 degrees
 Acq. time 1.891 sec
 Width 6025.9 Hz
 Arrayed repetitions
OBSERVE   H1, 499.9270453 MHz
DATA PROCESSING
FT size 32768
Total time 2 minutes
```

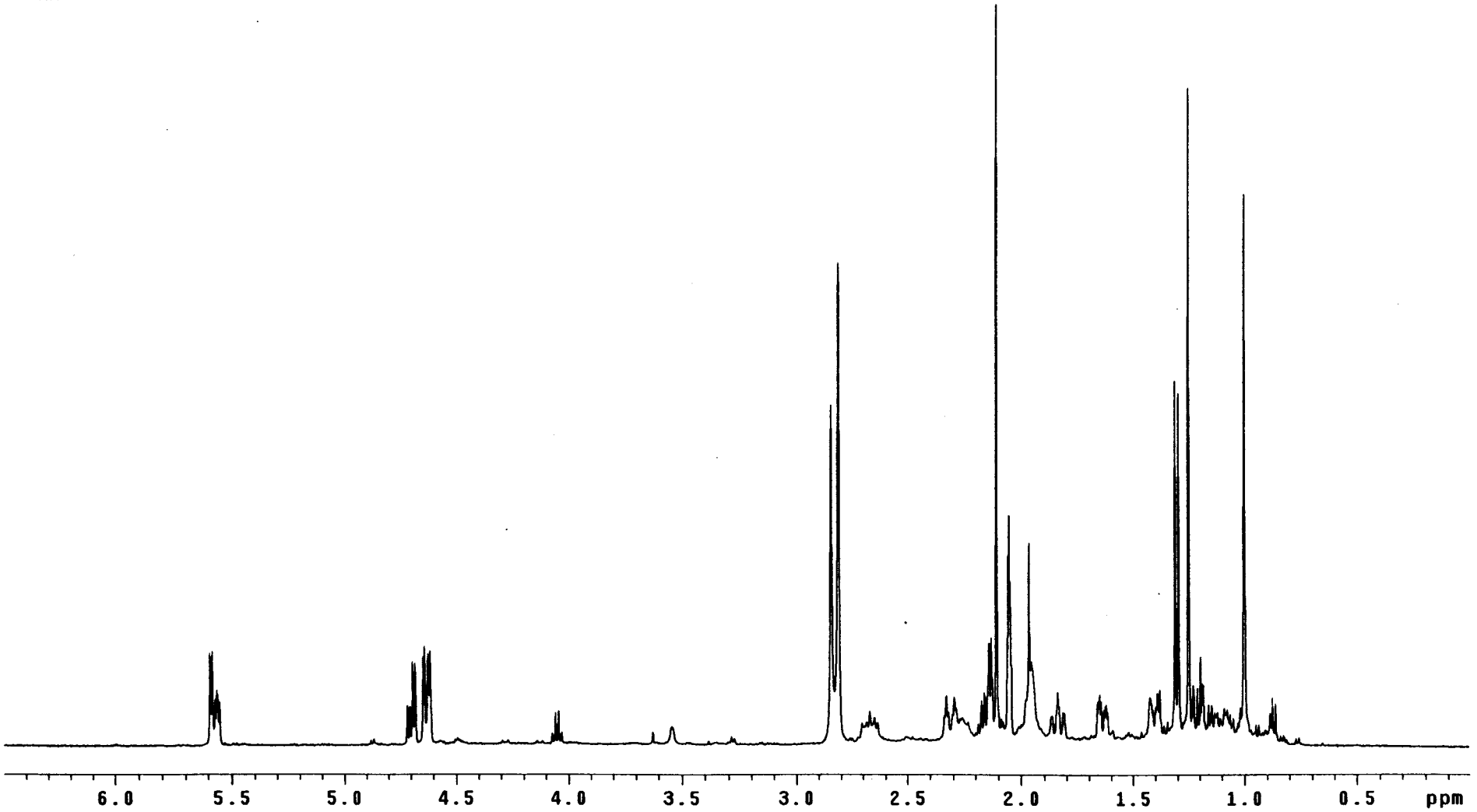
Guanacastepene I – ^{1}H NMR

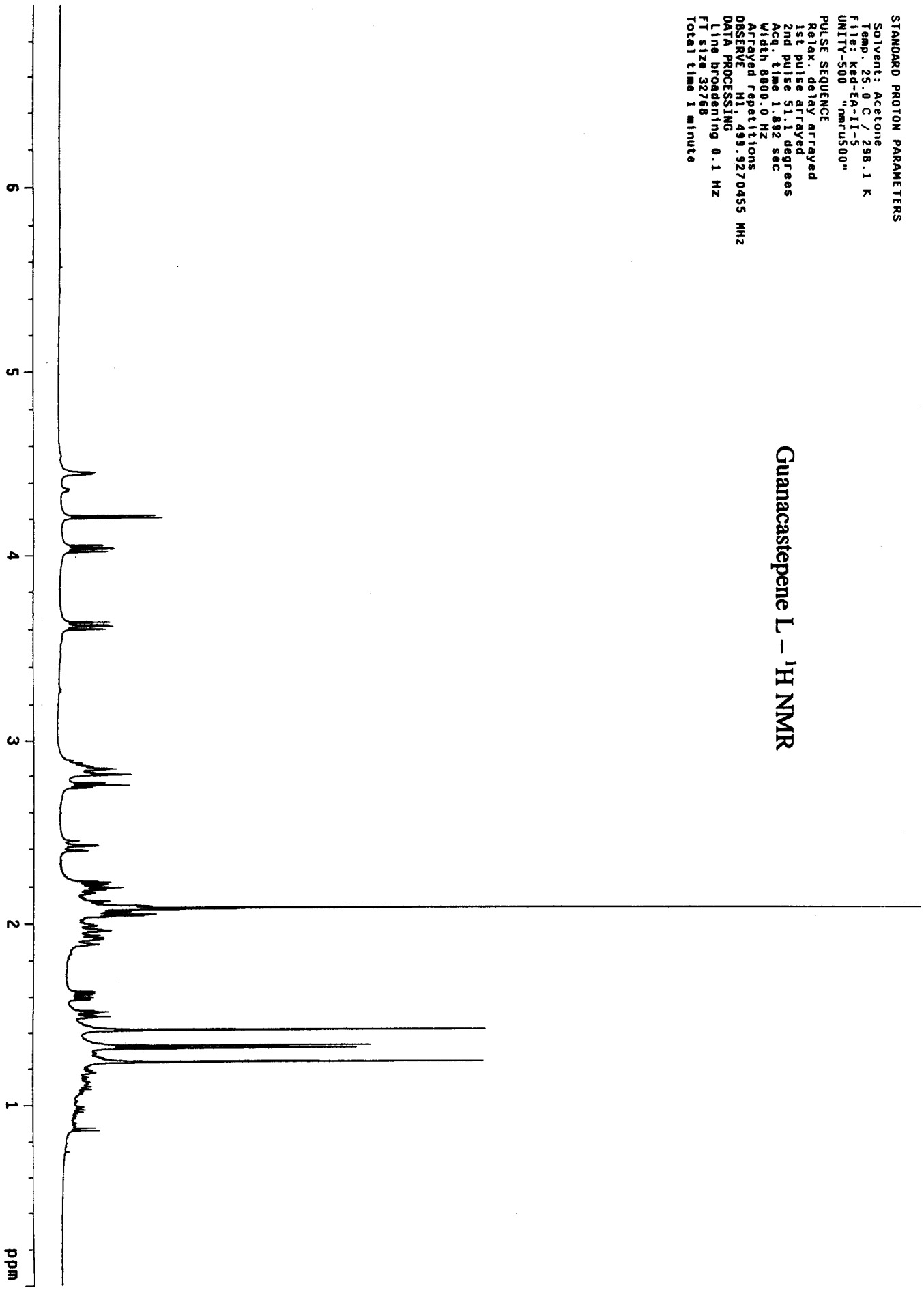



new experiment
Solvent: Acetone
Temp. -50.0 C / 223.2 K
File: cr115-8-h-50
INOVA-500 "workstation1"
PULSE SEQUENCE
Pulse 45.0 degrees
Acq. time 1.891 sec
Width 6025.9 Hz
86 repetitions
OBSERVE H1, 499.9270455 MHz
DATA PROCESSING
FT size 32768
Total time 2 minutes
Guanacastepene I – ^{1}H NMR
8
7
6
5
4
3
2
1
ppm

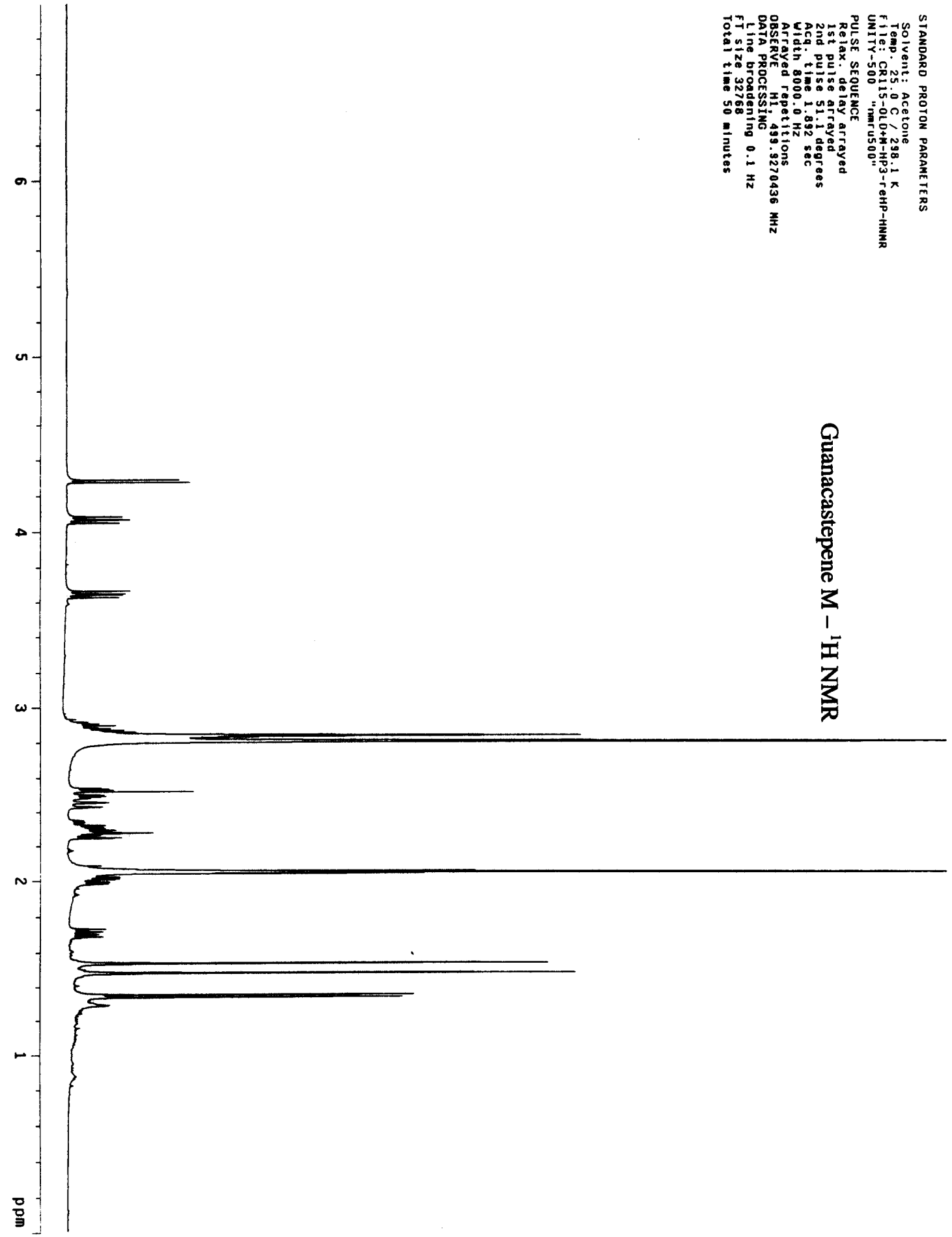
STANDARD PROTON PARAMETERS
Solvent: Acetone
Temp. 25.0 C / 298.1 K
File: KED-I-6-H
INOVA-500 "workstation1"
PULSE SEQUENCE
Pulse 51.1 degrees
Acq. time 1.891 sec
Width 3249.7 Hz
8 repetitions
OBSERVE H1, 499.9270441 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 16384
Total time 1 minute

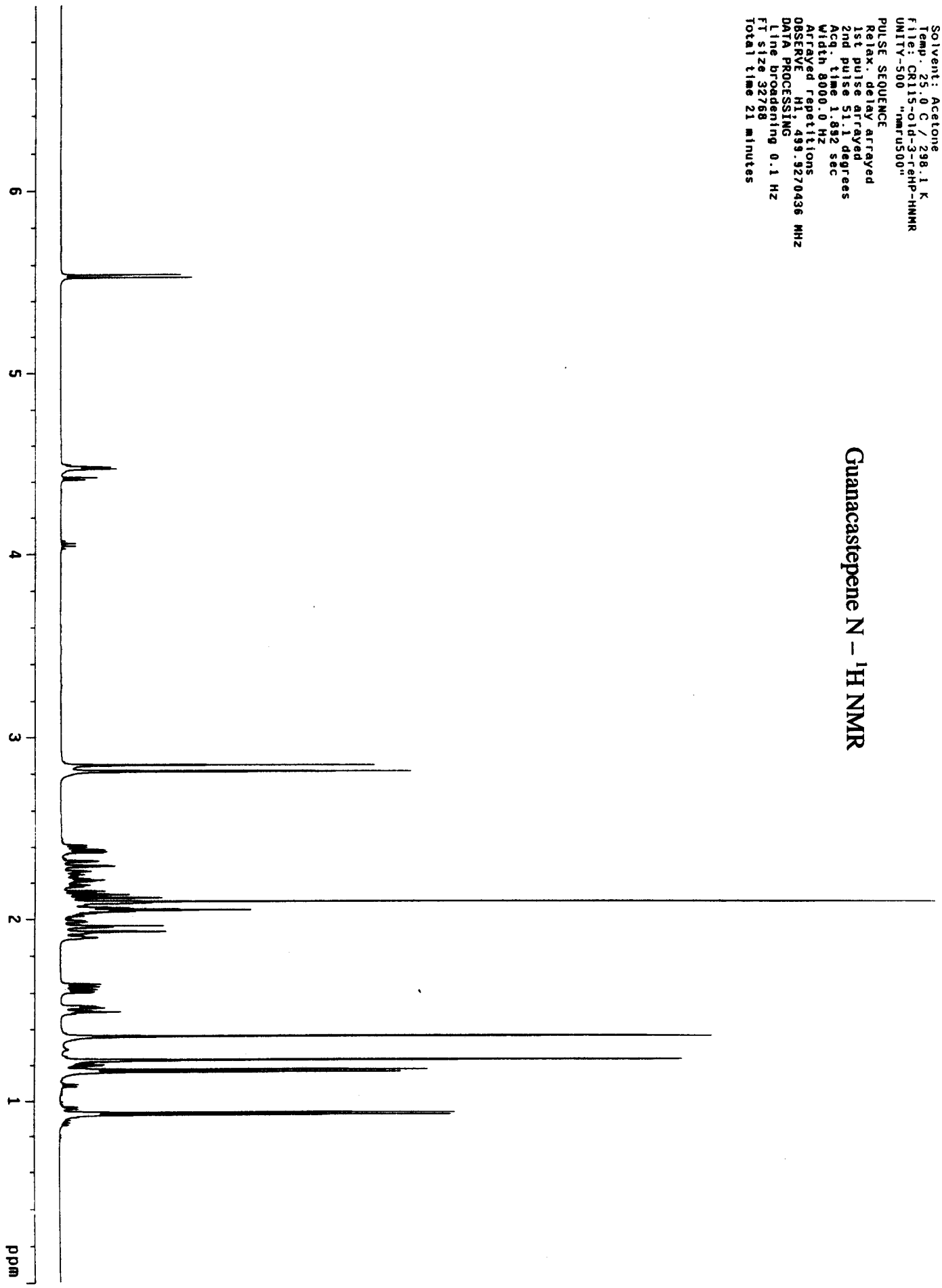
Guanacastepene K – ^{1}H NMR

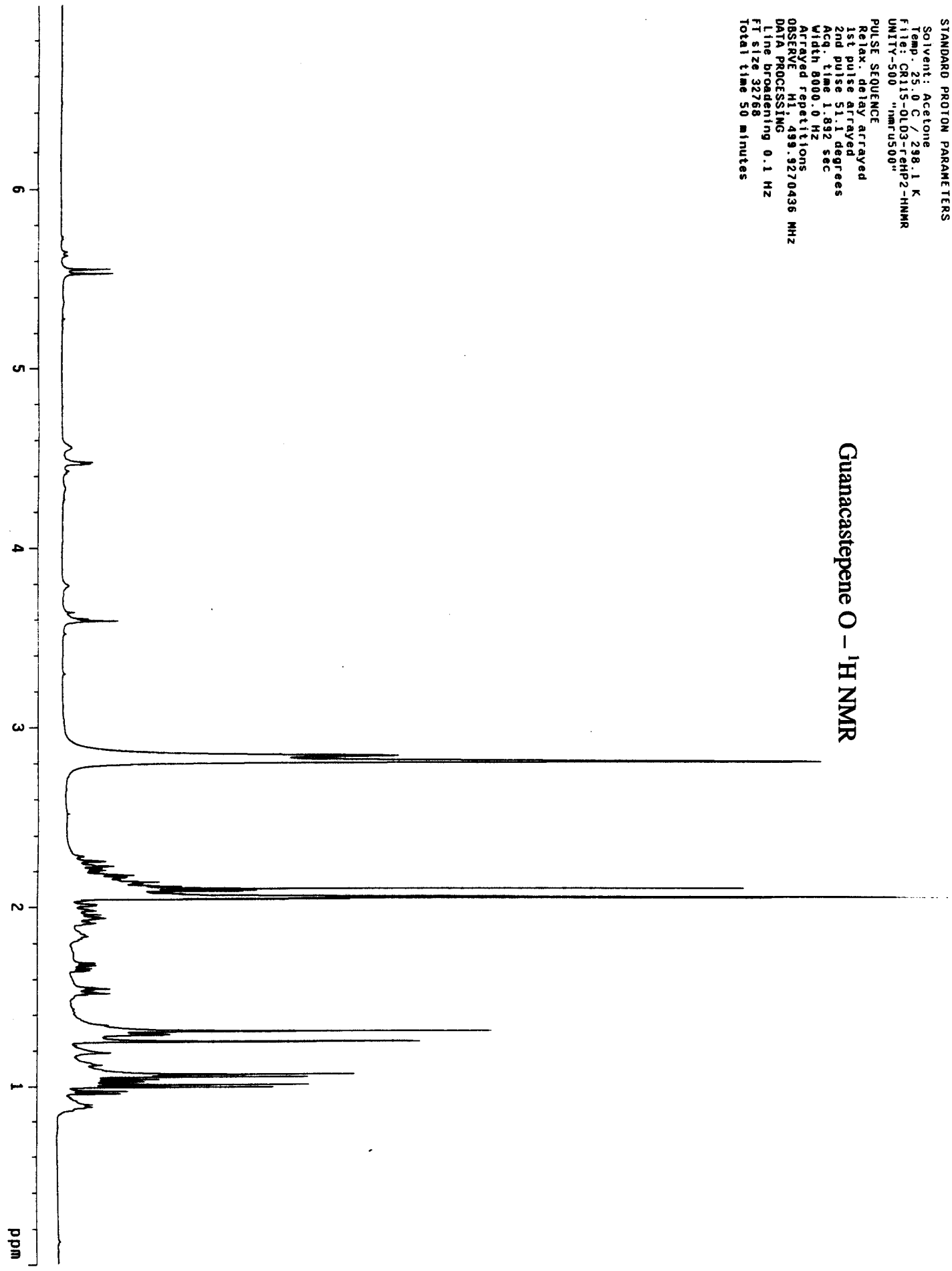




Guanacastepene L – ^{1}H NMR


STANDARD PROTON PARAMETERS
Solvent: Acetone
Temp. 25.0 C / 298.1 K
File: CR115-OLD+M-HP3-reHP-HNMR
UNITY-500 "rmru500"
PULSE SEQUENCE
Relax. delay arrayed
1st pulse arrayed
2nd pulse 51.1 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
Arrayed repetitions
OBSERVE H1, 499.9270436 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 50 minutes
Guanacastepene M – ^{1}H NMR
6
5
4
3
2
1
ppm


STANDARD PROTON PARAMETERS
Solvent: Acetone
Temp. 25.0 C / 298.1 K
File: CR115-old-3-reHP-HNMR
UNITY-500 "nmru500"
PULSE SEQUENCE
Relax. delay arrayed
1st pulse arrayed
2nd pulse 51.1 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
Arrayed repetitions
OBSERVE H1, 499.9270436 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 21 minutes
Guanacastepene N – ^{1}H NMR
6
5
4
3
2
1
ppm


STANDARD PROTON PARAMETERS
Solvent: Acetone
Temp. 25.0 C / 298.1 K
File: CR115-OLD3-reHP2-HNMR
UNITY-500 "nmru500"
PULSE SEQUENCE
Relax. delay arrayed
1st pulse arrayed
2nd pulse 51.1 degrees
Acq. time 1.892 sec
Width 8000.0 HZ
Arrayed repetitions
OBSERVE H1, 499.9270436 MHz
DATA PROCESSING
Line broadening 0.1 HZ
FT size 32768
Total time 50 minutes
Guanacastepene O – ^{1}H NMR
6
5
4
3
2
1
ppm