Supplementary Material

Unique cyclolignan's architecture obtained *via* acid catalyzed cyclization/intramolecular Friedel-Crafts tandem reaction

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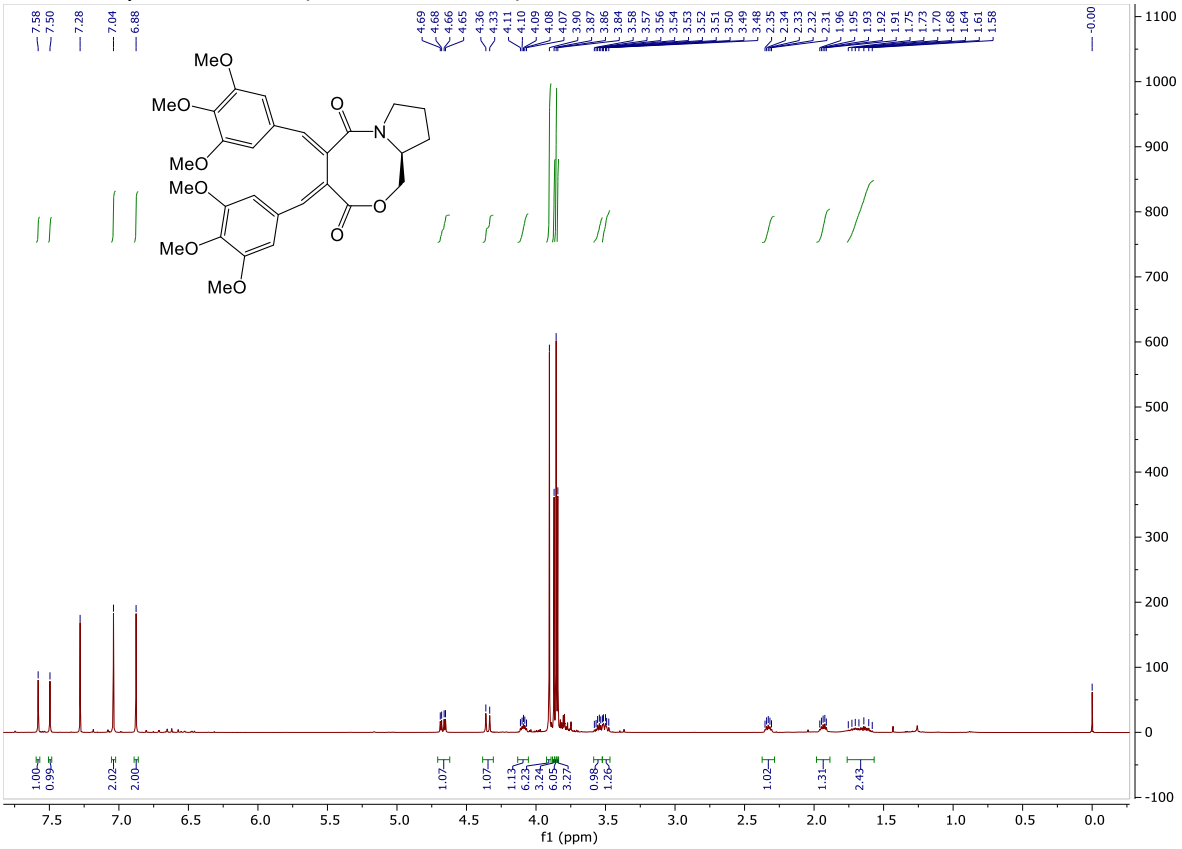
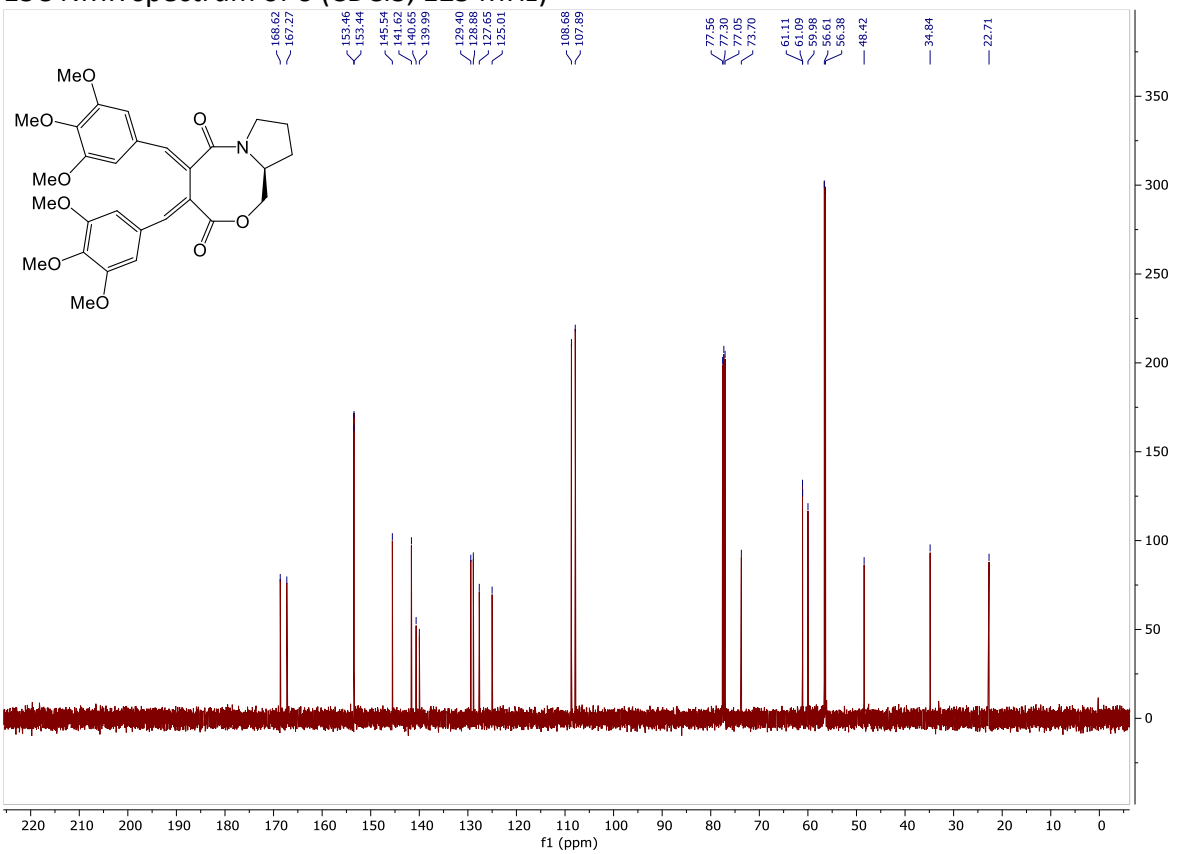
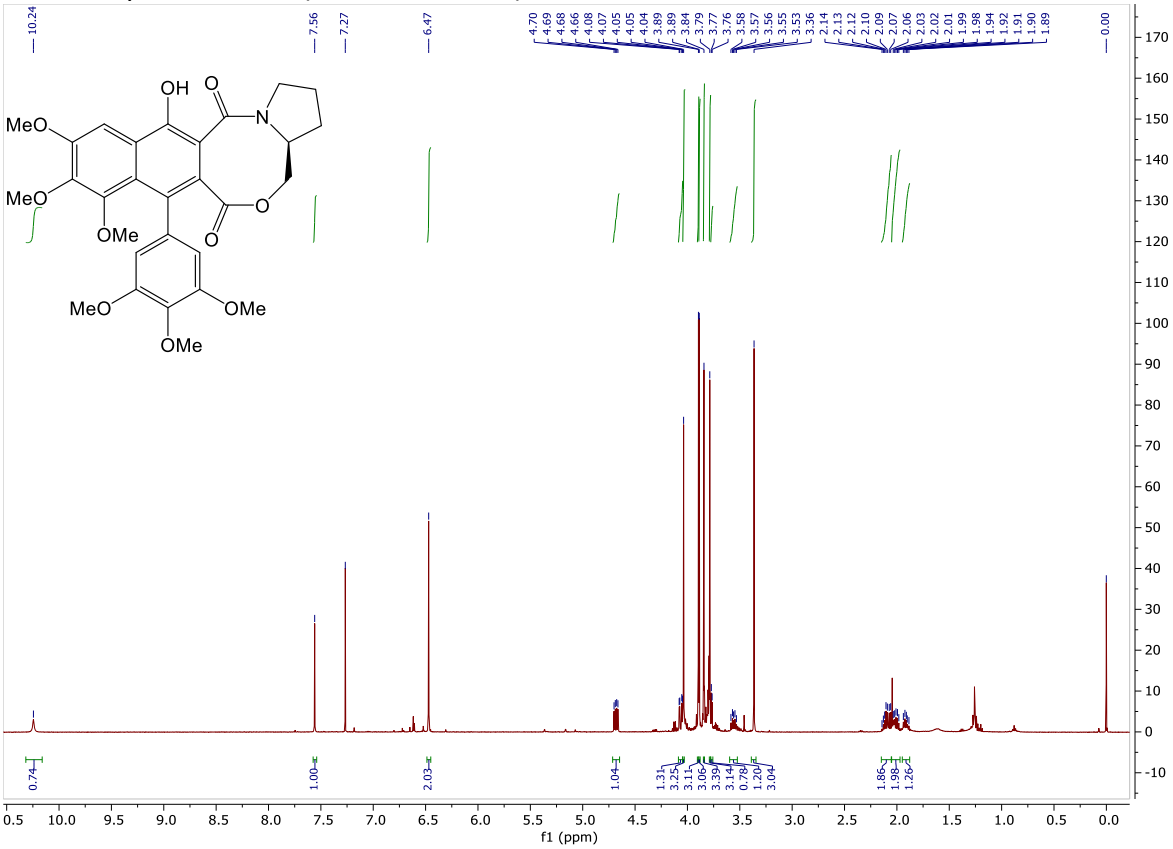
^{1}H NMR spectrum of **6** ($CDCl_3$, 500 MHz)



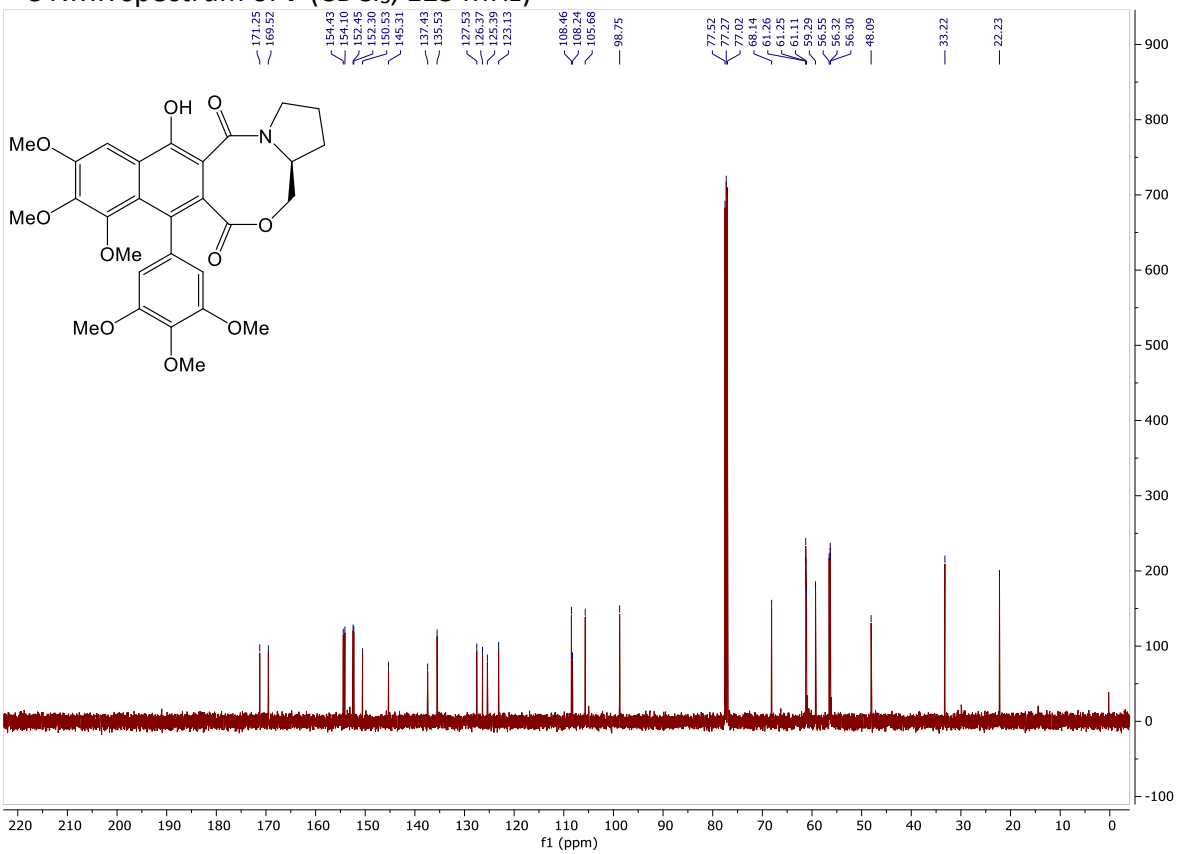
13C NMR spectrum of **6** (CDCl3, 125 MHz)



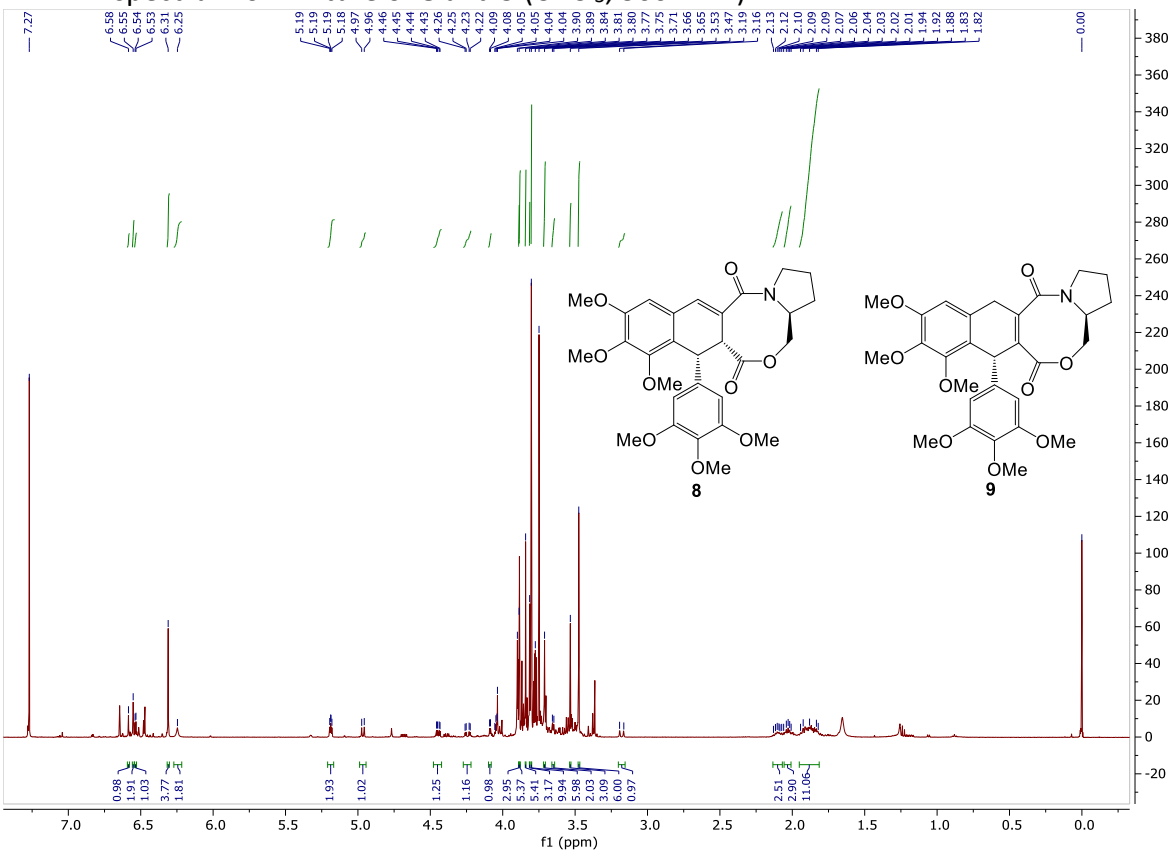
^{1}H NMR spectrum of **7** ($CDCl_3$, 500 MHz)



^{13}C NMR spectrum of **7** ($CDCl_3$, 125 MHz)



^{1}H NMR spectrum of mixture of **8** and **9** ($CDCl_3$, 500 MHz)



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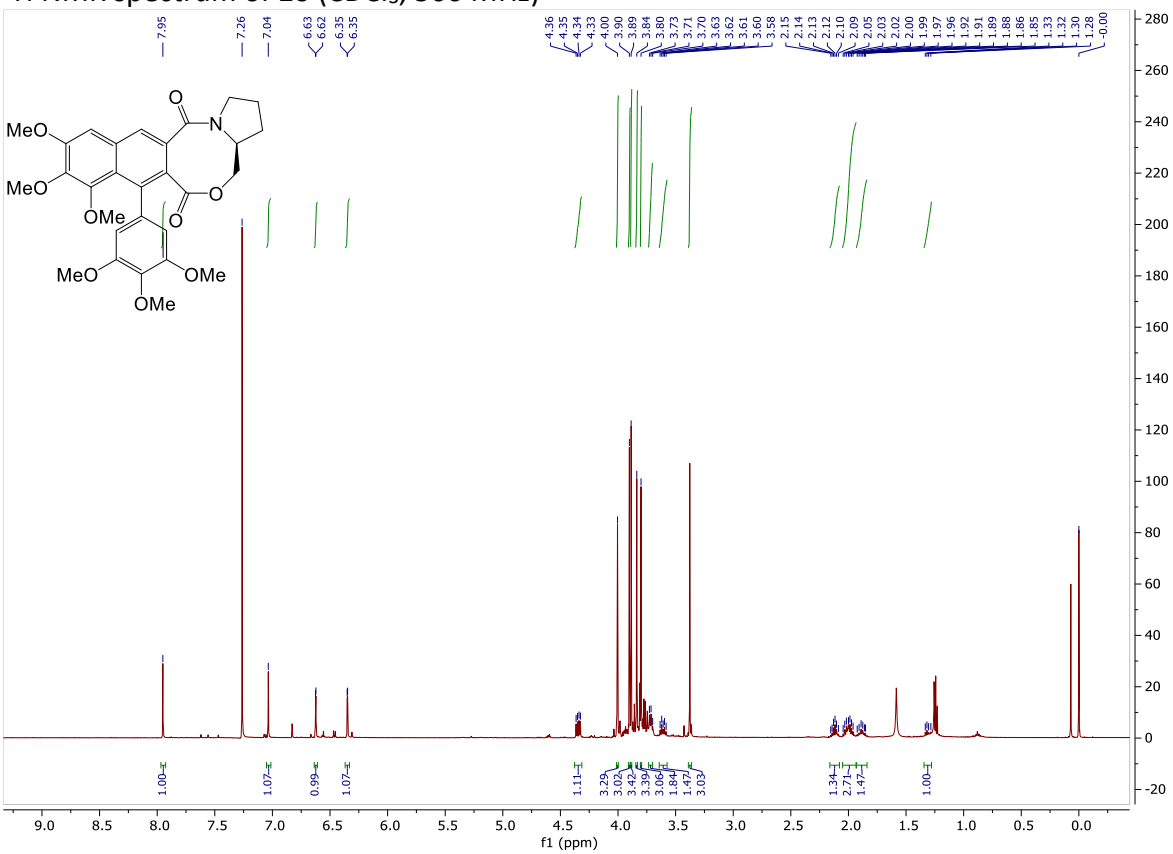

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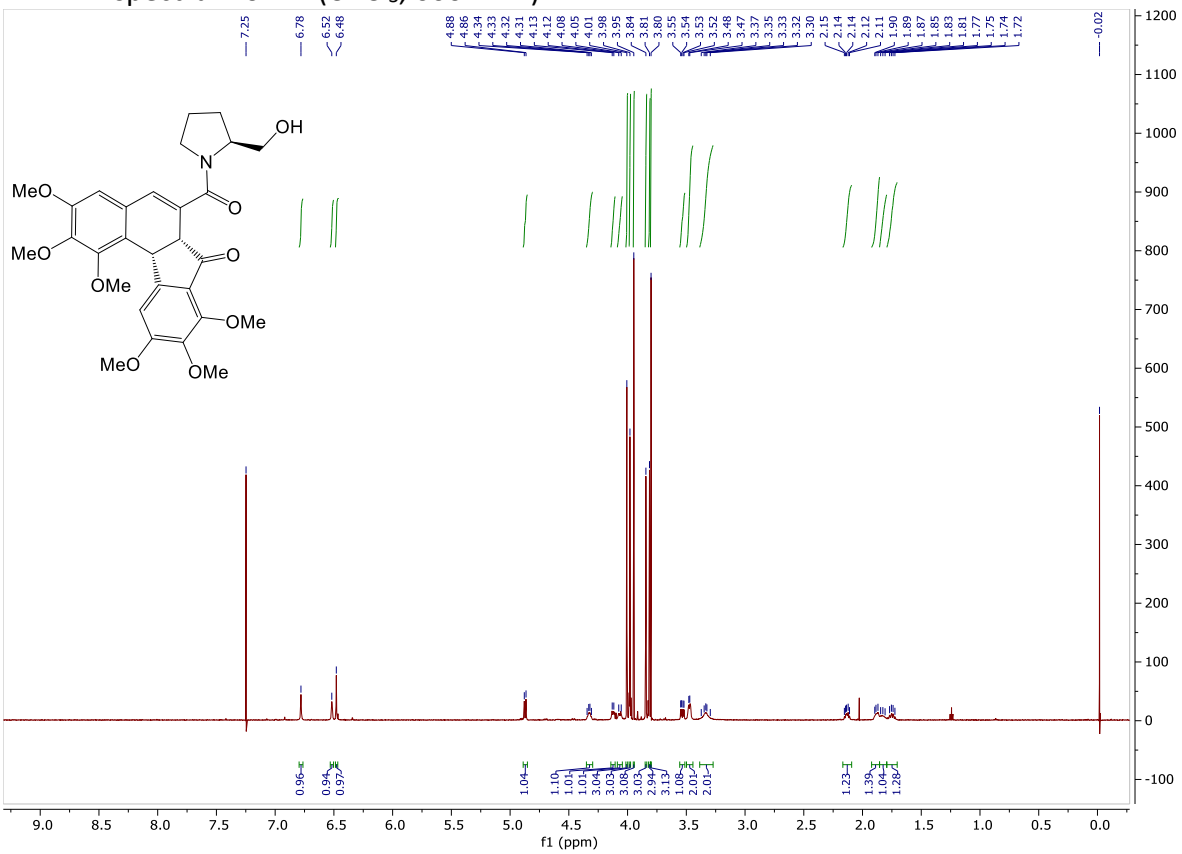
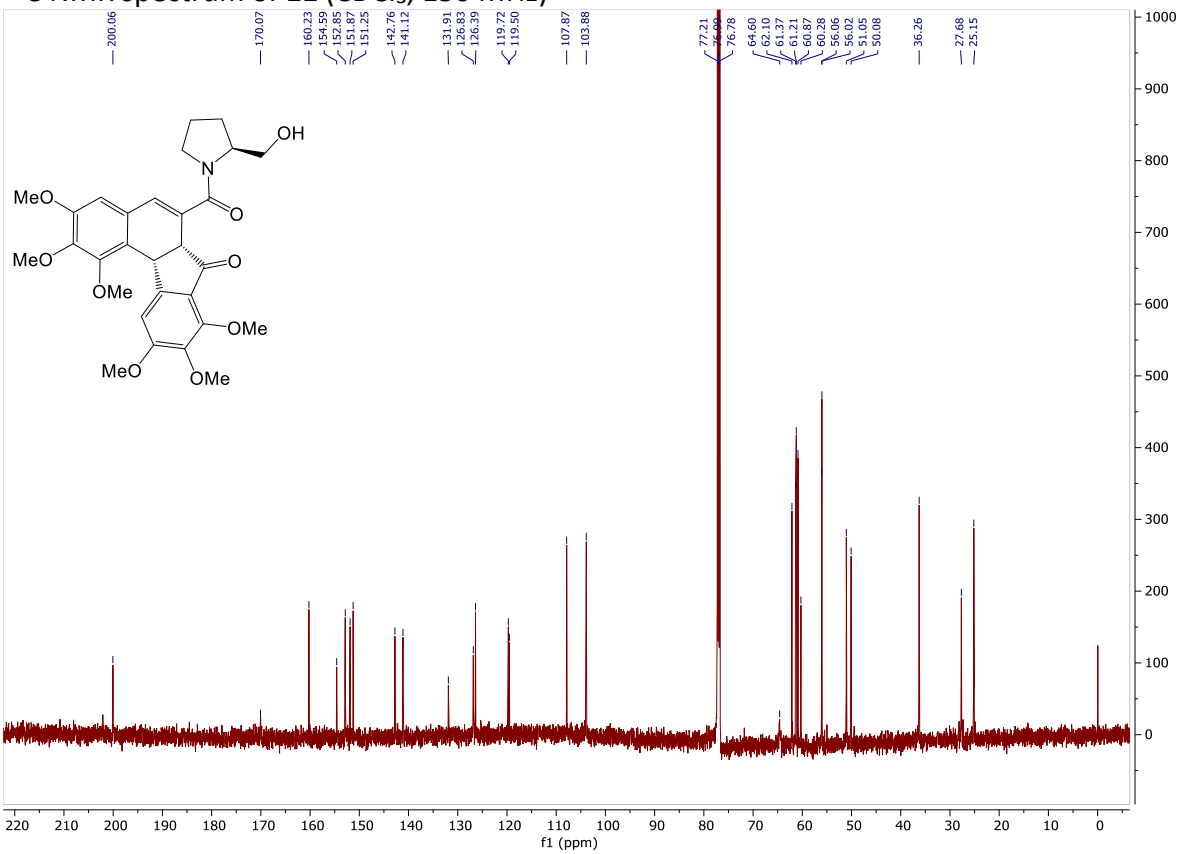
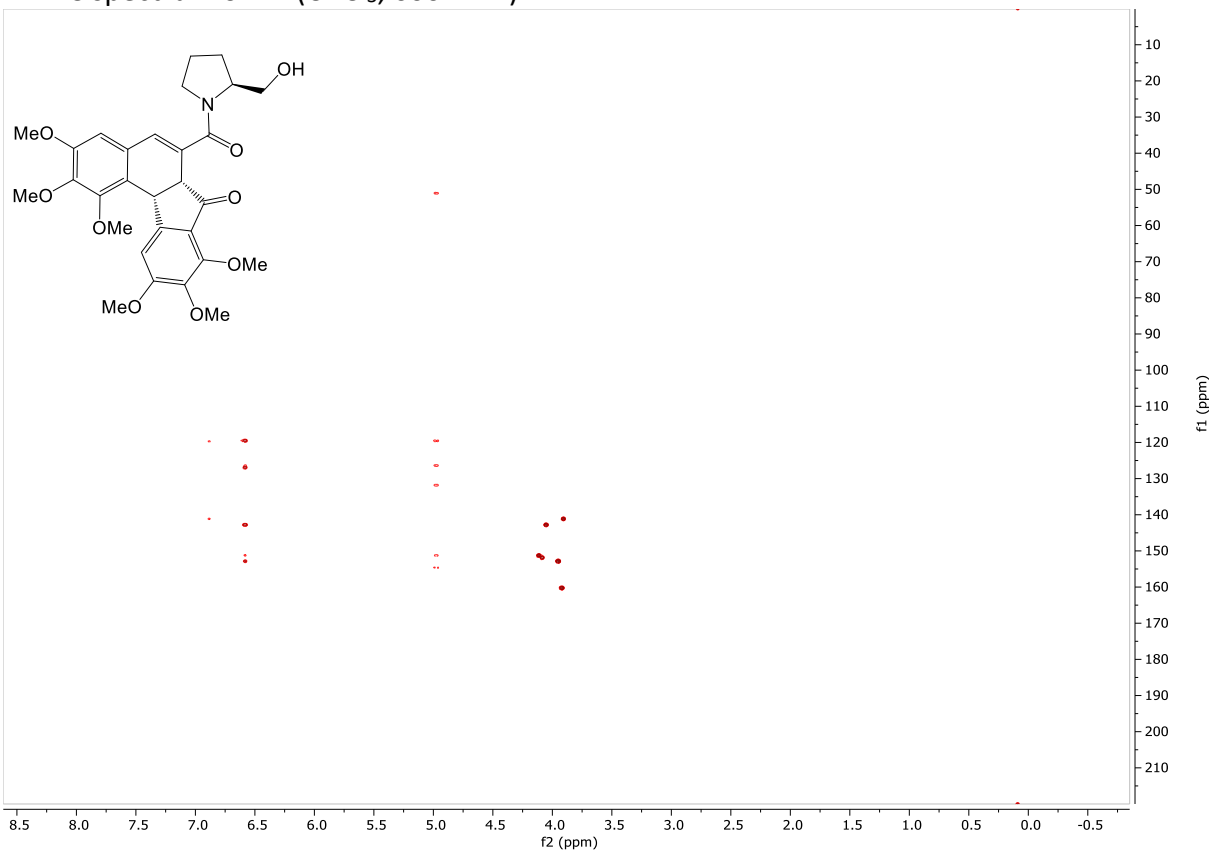


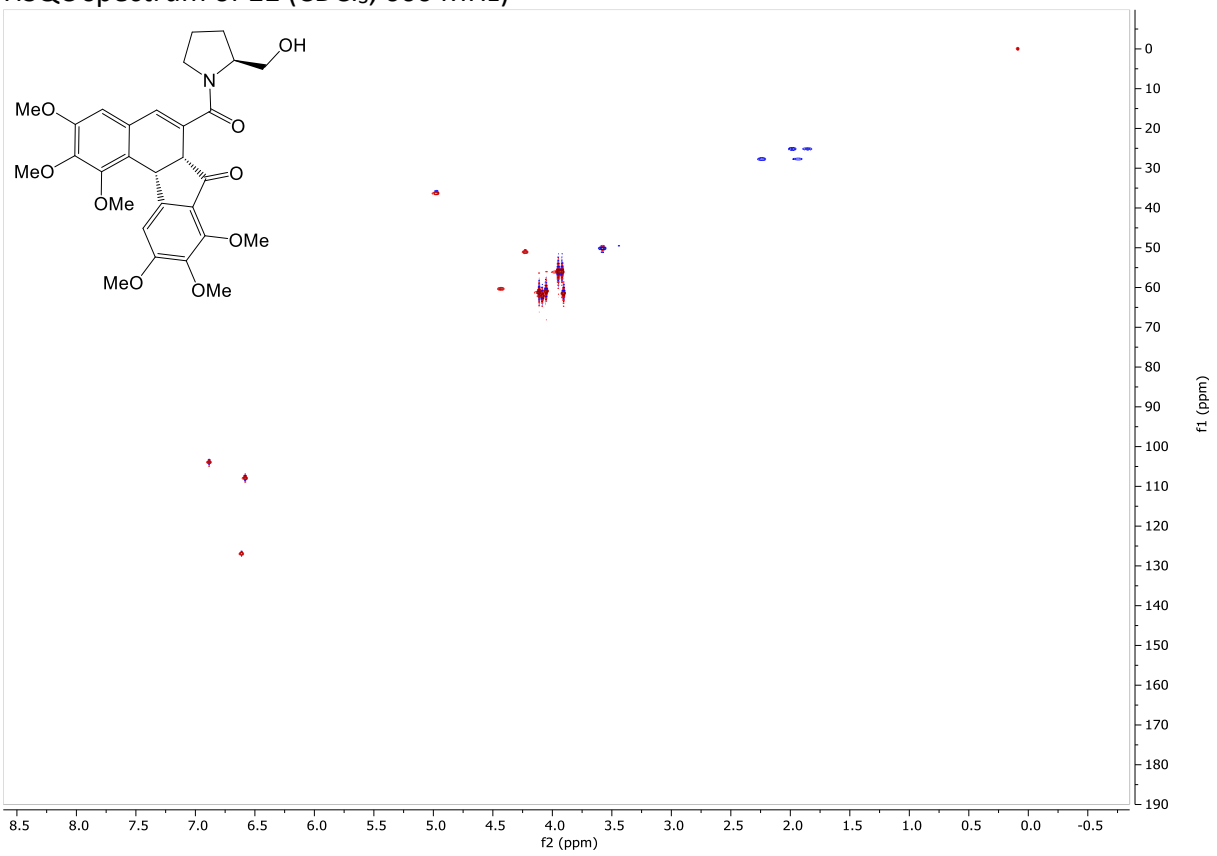
^{13}C NMR spectrum of **11** ($CDCl_3$, 150 MHz)



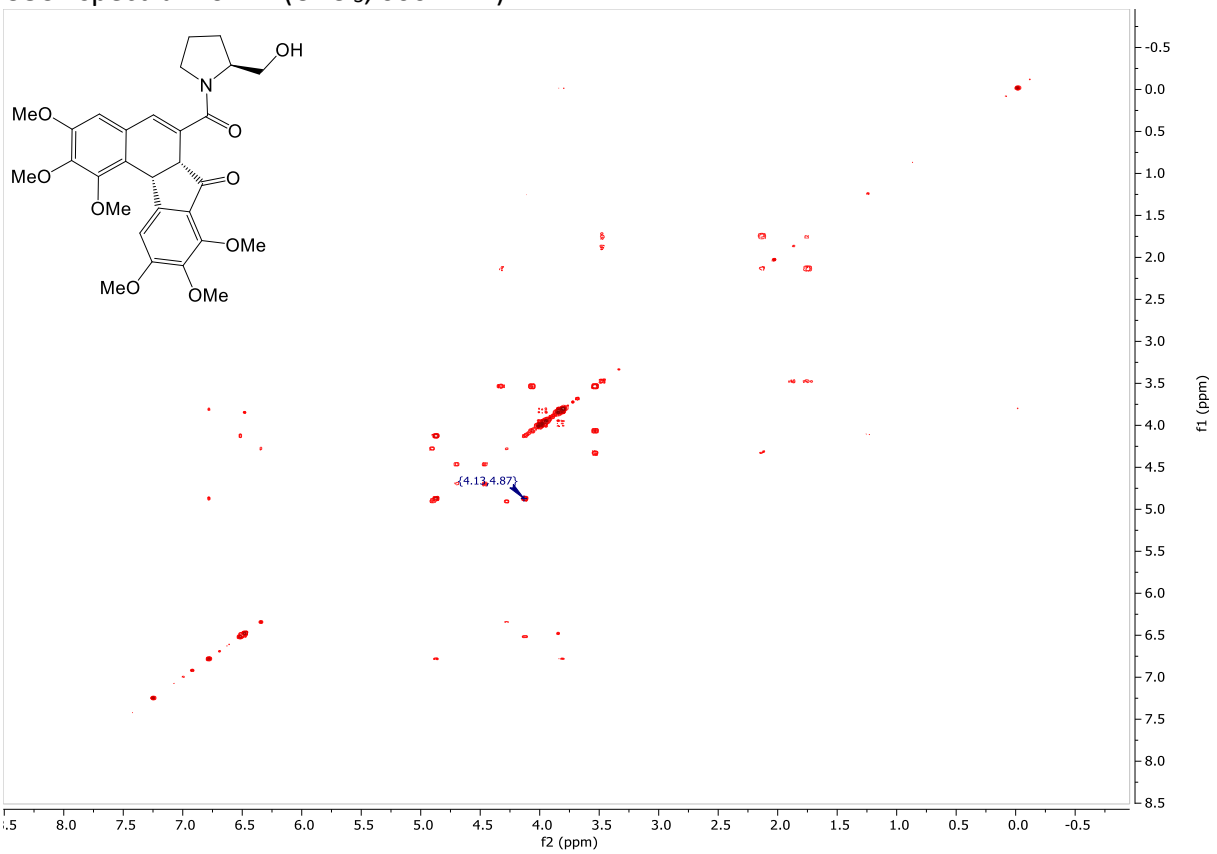
HMBC spectrum of **11** ($CDCl_3$, 600 MHz)



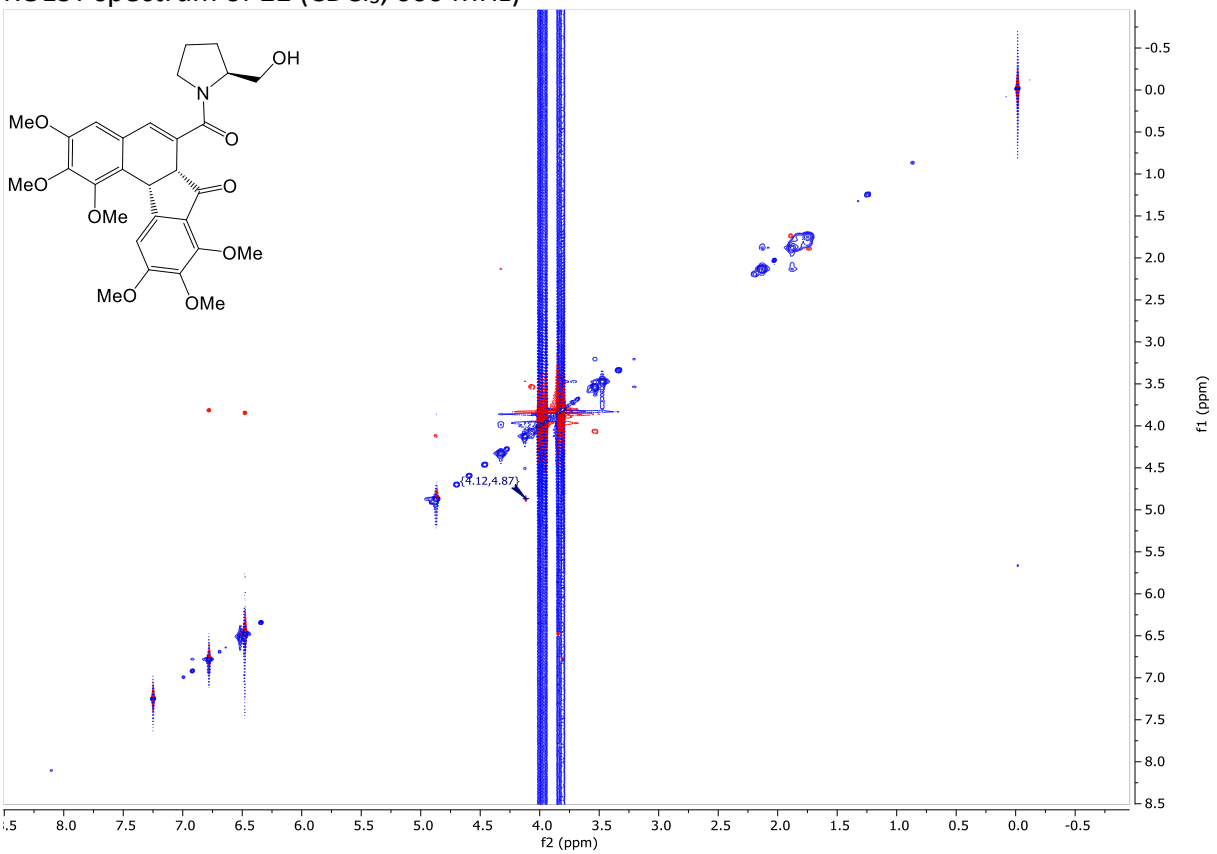
HSQC spectrum of **11** ($CDCl_3$, 600 MHz)



COSY spectrum of **11** ($CDCl_3$, 600 MHz)



ROESY spectrum of **11** ($CDCl_3$, 600 MHz)



Details of X-Ray Crystal Structure analysis for 11

The X-ray crystallographic experiment was performed using Oxford Diffraction Excalibur R single crystal diffractometer. The graphite-monochromatized Cu Kα radiation was applied. The preliminary experiment was used for calculation of unit cell dimensions and crystal symmetry assignment. Final experiment was then performed. Data were corrected for Lorenz-polarization effects and for absorption. Collected data were used for structure solution and refinement. Direct methods from SHELXS-97 and full matrix least-squares refinement from SHELXL-97 (G.M. Sheldrick, *Acta Cryst*. (2008). **A64**, 112–122) were applied for this purposes. To enable determination of an absolute structure all Friedel pairs were measured. During refinement correctness of the molecule configuration was verified using the Flack parameter (S. Parsons, P. Pattisonb, H.D. Flack, *Acta Cryst*. (2012). **A68**, 736–749) – the near-zero value correspond to a proper absolute structure and hence a proper enantiomer/diastereoisomer of the compound.

Crystal structure of **11**. A good quality colorless block shaped crystal of dimensions 0.4×0.07×0.02 mm was mounted on the diffractometer. 24068 reflections were collected of which 4849 were classified as independent after merging. The crystals of **11** crystallize in the acentrosymmetric orthorhombic $P2_12_12_1$ space group.

The experimental parameters for the structure are collected in Tables (*vide infra*). The conformation of the molecule is shown in Figure 1. The crystal packing is shown in Figure 2. The characteristic O-H···O hydrogen bonds are depicted as the dashed lines. The full experimental and structural parameters were deposited with Cambridge Structural Data Centre under the number **CCDC 1977939**.

Table 1. Crystal data and structure refinement for ZC171-1abs

Identification code	zc171-1abs
Deposit number	CCDC 1977939
Empirical formula	$C_{29}H_{32}NO_9$
Formula weight	538.56
Temperature	293(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	P $2_12_12_1$
Unit cell dimensions	a = 5.02660(10) Å, □= 90°
	b = 13.0853(2) Å, □= 90°
	c = 39.8047(9) Å, □ = 90°
Volume	2618.14(9) $Å^3$
Z	4
Density (calculated)	1.366 Mg/m^3
Absorption coefficient	0.846 mm^{-1}
F(000)	1140
Crystal size	0.3773 x 0.0721 x 0.0224 mm^3
Theta range for data collection	3.56 to 70.37°
Index ranges	-5≤h≤5, -15≤k≤15, -48≤l≤47
Reflections collected	24068
Independent reflections	4849 [R(int) = 0.0590]

Completeness to theta = 70.37°	97.9 %
Absorption correction	Analytical
Max. and min. transmission	0.981 and 0.838
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4849 / 0 / 355
Goodness-of-fit on F^2	0.840
Final R indices [I>2σ(I)]	R1 = 0.0381, wR2 = 0.0790
R indices (all data)	R1 = 0.0688, wR2 = 0.0862
Absolute structure parameter	-0.1(2)
Largest diff. peak and hole	0.159 and -0.167 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for ZC171-1abs. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
O(1)	6832(4)	2111(1)	9282(1)	67(1)
O(2)	6734(4)	3760(1)	8506(1)	56(1)
O(3)	9981(4)	923(1)	9802(1)	62(1)
O(4)	13210(5)	-791(1)	9863(1)	71(1)
O(5)	14682(5)	-1834(1)	9324(1)	71(1)
O(6)	9261(4)	-1413(1)	8254(1)	70(1)
O(7)	12312(4)	-1551(1)	7655(1)	60(1)
O(8)	15188(5)	57(1)	7457(1)	67(1)
C(1)	7909(5)	1472(2)	9107(1)	48(1)
C(2)	9610(5)	618(2)	9208(1)	44(1)
C(3)	10615(6)	352(2)	9525(1)	51(1)
C(4)	12242(6)	-492(2)	9555(1)	56(1)
C(5)	13003(6)	-1041(2)	9266(1)	53(1)
C(6)	11991(6)	-789(2)	8952(1)	48(1)
C(7)	10248(5)	27(2)	8928(1)	44(1)
C(8)	8757(6)	386(2)	8617(1)	45(1)
C(9)	10370(5)	321(2)	8302(1)	43(1)
C(10)	10564(5)	-589(2)	8118(1)	47(1)
C(11)	12096(6)	-642(2)	7828(1)	48(1)
C(12)	13626(6)	202(2)	7733(1)	50(1)
C(13)	13482(6)	1103(2)	7912(1)	47(1)
C(14)	11814(5)	1170(2)	8193(1)	42(1)
C(15)	11399(5)	2152(2)	8361(1)	43(1)
C(16)	9465(5)	2313(2)	8583(1)	43(1)
C(17)	7770(5)	1465(2)	8720(1)	44(1)
C(18)	8685(6)	3404(2)	8656(1)	45(1)
N(19)	10254(5)	3966(1)	8853(1)	50(1)
C(20)	12140(6)	3565(2)	9102(1)	63(1)
C(21)	12172(11)	4336(2)	9364(1)	120(2)
C(22)	11177(8)	5289(2)	9235(1)	76(1)
C(23)	9778(6)	5074(2)	8903(1)	53(1)
C(24)	12061(7)	1562(2)	9915(1)	80(1)
C(25)	11347(9)	-1390(3)	10044(1)	109(1)
C(26)	15847(6)	-2333(2)	9045(1)	68(1)
C(27)	7805(8)	-2095(2)	8056(1)	81(1)
C(28)	11236(8)	-1532(2)	7319(1)	77(1)
C(29)	16838(8)	878(2)	7350(1)	76(1)
C(30)	10785(6)	5671(2)	8605(1)	64(1)

O(9)	13617(5)	5639(1)	8562(1)	75(1)

Table 3. Bond lengths [Å] and angles [°] for ZC171-1abs

O(1)-C(1)	1.214(3)
O(2)-C(18)	1.240(3)
O(3)-C(3)	1.366(3)
O(3)-C(24)	1.412(4)
O(4)-C(4)	1.378(3)
O(4)-C(25)	1.418(4)
O(5)-C(5)	1.358(3)
O(5)-C(26)	1.416(3)
O(6)-C(10)	1.373(3)
O(6)-C(27)	1.397(3)
O(7)-C(11)	1.378(3)
O(7)-C(28)	1.444(3)
O(8)-C(12)	1.362(3)
O(8)-C(29)	1.423(4)
C(1)-C(2)	1.464(3)
C(1)-C(17)	1.543(3)
C(2)-C(7)	1.393(3)
C(2)-C(3)	1.404(3)
C(3)-C(4)	1.379(3)
C(4)-C(5)	1.408(3)
C(5)-C(6)	1.387(3)
C(6)-C(7)	1.384(3)
C(6)-H(6)	0.9300
C(7)-C(8)	1.522(3)
C(8)-C(9)	1.497(3)
C(8)-C(17)	1.551(3)
C(8)-H(8)	0.9800
C(9)-C(14)	1.396(3)
C(9)-C(10)	1.400(3)
C(10)-C(11)	1.390(3)
C(11)-C(12)	1.399(4)
C(12)-C(13)	1.379(3)
C(13)-C(14)	1.402(3)
C(13)-H(13)	0.9300
C(14)-C(15)	1.462(3)
C(15)-C(16)	1.332(3)

C(15)-H(15)	0.9300
C(16)-C(17)	1.501(3)
C(16)-C(18)	1.508(3)
C(17)-H(17)	0.9800
C(18)-N(19)	1.333(3)
N(19)-C(20)	1.470(3)
N(19)-C(23)	1.483(3)
C(20)-C(21)	1.449(4)
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(21)-C(22)	1.439(4)
C(21)-H(21)	0.9300
C(22)-C(23)	1.523(4)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-C(30)	1.507(4)
C(23)-H(23)	0.9800
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
C(30)-O(9)	1.434(4)
C(30)-H(30A)	0.9700
C(30)-H(30B)	0.9700
O(9)-H(9)	0.96(4)

C(3)-O(3)-C(24)	114.1(2)
C(4)-O(4)-C(25)	112.1(3)
C(5)-O(5)-C(26)	118.4(2)
C(10)-O(6)-C(27)	122.0(2)

C(11)-O(7)-C(28)	114.71(18)
C(12)-O(8)-C(29)	118.16(19)
O(1)-C(1)-C(2)	129.0(2)
O(1)-C(1)-C(17)	123.8(2)
C(2)-C(1)-C(17)	107.2(2)
C(7)-C(2)-C(3)	119.9(2)
C(7)-C(2)-C(1)	109.8(2)
C(3)-C(2)-C(1)	130.3(2)
O(3)-C(3)-C(4)	120.6(2)
O(3)-C(3)-C(2)	120.3(2)
C(4)-C(3)-C(2)	119.1(2)
O(4)-C(4)-C(3)	120.8(2)
O(4)-C(4)-C(5)	119.1(2)
C(3)-C(4)-C(5)	120.1(2)
O(5)-C(5)-C(6)	124.3(2)
O(5)-C(5)-C(4)	114.8(2)
C(6)-C(5)-C(4)	120.9(2)
C(7)-C(6)-C(5)	118.5(2)
C(7)-C(6)-H(6)	120.8
C(5)-C(6)-H(6)	120.8
C(6)-C(7)-C(2)	121.2(2)
C(6)-C(7)-C(8)	127.3(2)
C(2)-C(7)-C(8)	111.4(2)
C(9)-C(8)-C(7)	113.5(2)
C(9)-C(8)-C(17)	116.44(17)
C(7)-C(8)-C(17)	103.00(17)
C(9)-C(8)-H(8)	107.8
C(7)-C(8)-H(8)	107.8
C(17)-C(8)-H(8)	107.8
C(14)-C(9)-C(10)	118.6(2)
C(14)-C(9)-C(8)	119.76(19)
C(10)-C(9)-C(8)	121.6(2)
O(6)-C(10)-C(11)	123.5(2)
O(6)-C(10)-C(9)	115.4(2)
C(11)-C(10)-C(9)	121.0(2)
O(7)-C(11)-C(10)	120.1(2)
O(7)-C(11)-C(12)	120.2(2)
C(10)-C(11)-C(12)	119.4(2)
O(8)-C(12)-C(13)	124.5(2)
O(8)-C(12)-C(11)	115.2(2)
C(13)-C(12)-C(11)	120.3(2)
C(12)-C(13)-C(14)	119.9(2)
C(12)-C(13)-H(13)	120.0
C(14)-C(13)-H(13)	120.0

C(9)-C(14)-C(13)	120.5(2)
C(9)-C(14)-C(15)	118.9(2)
C(13)-C(14)-C(15)	120.3(2)
C(16)-C(15)-C(14)	123.1(2)
C(16)-C(15)-H(15)	118.4
C(14)-C(15)-H(15)	118.4
C(15)-C(16)-C(17)	122.5(2)
C(15)-C(16)-C(18)	117.9(2)
C(17)-C(16)-C(18)	118.9(2)
C(16)-C(17)-C(1)	109.37(19)
C(16)-C(17)-C(8)	113.3(2)
C(1)-C(17)-C(8)	104.70(17)
C(16)-C(17)-H(17)	109.8
C(1)-C(17)-H(17)	109.8
C(8)-C(17)-H(17)	109.8
O(2)-C(18)-N(19)	123.0(2)
O(2)-C(18)-C(16)	118.0(2)
N(19)-C(18)-C(16)	118.7(2)
C(18)-N(19)-C(20)	125.60(19)
C(18)-N(19)-C(23)	121.5(2)
C(20)-N(19)-C(23)	111.28(19)
C(21)-C(20)-N(19)	104.1(2)
C(21)-C(20)-H(20A)	110.9
N(19)-C(20)-H(20A)	110.9
C(21)-C(20)-H(20B)	110.9
N(19)-C(20)-H(20B)	110.9
H(20A)-C(20)-H(20B)	109.0
C(22)-C(21)-C(20)	110.1(2)
C(22)-C(21)-H(21)	125.0
C(20)-C(21)-H(21)	125.0
C(21)-C(22)-C(23)	108.1(2)
C(21)-C(22)-H(22A)	110.1
C(23)-C(22)-H(22A)	110.1
C(21)-C(22)-H(22B)	110.1
C(23)-C(22)-H(22B)	110.1
H(22A)-C(22)-H(22B)	108.4
N(19)-C(23)-C(30)	110.4(2)
N(19)-C(23)-C(22)	102.8(2)
C(30)-C(23)-C(22)	115.5(2)
N(19)-C(23)-H(23)	109.3
C(30)-C(23)-H(23)	109.3
C(22)-C(23)-H(23)	109.3
O(3)-C(24)-H(24A)	109.5
O(3)-C(24)-H(24B)	109.5

H(24A)-C(24)-H(24B)	109.5
O(3)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
O(4)-C(25)-H(25A)	109.5
O(4)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
O(4)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
O(5)-C(26)-H(26A)	109.5
O(5)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
O(5)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
O(6)-C(27)-H(27A)	109.5
O(6)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
O(6)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
O(7)-C(28)-H(28A)	109.5
O(7)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
O(7)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
O(8)-C(29)-H(29A)	109.5
O(8)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
O(8)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
O(9)-C(30)-C(23)	114.3(2)
O(9)-C(30)-H(30A)	108.7
C(23)-C(30)-H(30A)	108.7
O(9)-C(30)-H(30B)	108.7
C(23)-C(30)-H(30B)	108.7
H(30A)-C(30)-H(30B)	107.6
C(30)-O(9)-H(9)	106(2)

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for ZC171-1abs. 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)	80(2)	65(1)	56(1)	-5(1)	6(1)	28(1)
O(2)	57(1)	47(1)	63(1)	-1(1)	-14(1)	10(1)
O(3)	72(1)	67(1)	47(1)	-11(1)	4(1)	6(1)
O(4)	89(2)	74(1)	51(1)	9(1)	-9(1)	17(1)
O(5)	95(2)	60(1)	57(1)	4(1)	-6(1)	29(1)
O(6)	106(2)	49(1)	54(1)	-5(1)	-3(1)	-26(1)
O(7)	87(2)	42(1)	51(1)	-13(1)	-8(1)	8(1)
O(8)	86(2)	55(1)	61(1)	-10(1)	16(1)	1(1)
C(1)	50(2)	47(1)	48(1)	-1(1)	5(1)	0(1)
C(2)	52(2)	38(1)	42(1)	0(1)	3(1)	0(1)
C(3)	62(2)	51(1)	42(1)	-2(1)	5(1)	3(1)
C(4)	75(2)	49(1)	43(1)	4(1)	-3(1)	7(1)
C(5)	67(2)	42(1)	51(2)	5(1)	-5(2)	10(1)
C(6)	64(2)	37(1)	44(1)	-4(1)	2(1)	2(1)
C(7)	54(2)	36(1)	43(1)	4(1)	-1(1)	-4(1)
C(8)	51(2)	39(1)	44(1)	-1(1)	-4(1)	-8(1)
C(9)	48(2)	41(1)	40(1)	-1(1)	-8(1)	1(1)
C(10)	59(2)	38(1)	43(1)	0(1)	-5(1)	-4(1)
C(11)	64(2)	35(1)	46(1)	-8(1)	-8(1)	8(1)
C(12)	59(2)	49(1)	41(1)	-4(1)	4(1)	7(1)
C(13)	52(2)	39(1)	49(1)	0(1)	1(1)	-2(1)
C(14)	46(2)	38(1)	41(1)	1(1)	-6(1)	0(1)
C(15)	49(2)	39(1)	43(1)	-2(1)	-5(1)	-1(1)
C(16)	46(2)	39(1)	43(1)	-2(1)	-6(1)	8(1)
C(17)	46(2)	45(1)	43(1)	0(1)	-3(1)	2(1)
C(18)	53(2)	43(1)	40(1)	2(1)	3(1)	6(1)
N(19)	59(2)	40(1)	50(1)	-7(1)	-11(1)	9(1)
C(20)	66(2)	57(2)	64(2)	-2(1)	-15(2)	10(2)
C(21)	218(5)	69(2)	73(2)	-22(2)	-72(3)	38(3)
C(22)	105(3)	61(2)	61(2)	-22(1)	-12(2)	5(2)
C(23)	57(2)	41(1)	59(2)	-10(1)	1(2)	6(1)
C(24)	96(3)	73(2)	69(2)	-17(2)	6(2)	-9(2)
C(25)	149(4)	107(2)	71(2)	34(2)	4(3)	-5(3)
C(26)	80(2)	47(1)	76(2)	-1(1)	0(2)	15(2)
C(27)	92(3)	67(2)	84(2)	-17(2)	-10(2)	-23(2)
C(28)	116(3)	65(2)	52(2)	-17(1)	-14(2)	-1(2)
C(29)	96(3)	62(2)	70(2)	5(1)	26(2)	5(2)
C(30)	74(3)	45(1)	74(2)	-1(1)	-10(2)	7(1)
O(9)	70(2)	52(1)	103(2)	-1(1)	12(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for ZC171-1abs

	x	y	z	U(eq)
H(6)	12472	-1160	8763	58
H(8)	7193	-53	8589	54
H(13)	14490	1664	7846	56
H(15)	12539	2689	8309	52
H(17)	5924	1558	8647	53
H(20A)	11542	2913	9190	75
H(20B)	13895	3480	9005	75
H(21)	12751	4230	9583	144
H(22A)	12633	5764	9200	91
H(22B)	9939	5591	9393	91
H(23)	7865	5195	8929	63
H(24A)	11480	1936	10109	119
H(24B)	12540	2032	9740	119
H(24C)	13576	1152	9973	119
H(25A)	12099	-1583	10257	163
H(25B)	10926	-1993	9918	163
H(25C)	9756	-1000	10081	163
H(26A)	16974	-2876	9122	101
H(26B)	16884	-1852	8918	101
H(26C)	14471	-2609	8904	101
H(27A)	7017	-2608	8197	121
H(27B)	8968	-2415	7896	121
H(27C)	6431	-1731	7939	121
H(28A)	11453	-2192	7217	116
H(28B)	12160	-1029	7188	116
H(28C)	9378	-1364	7328	116
H(29A)	17828	673	7155	114
H(29B)	18046	1058	7527	114
H(29C)	15750	1458	7295	114
H(30A)	9949	5407	8403	77
H(30B)	10241	6378	8630	77
H(9)	14060(70)	4940(30)	8520(8)	112

Table 6. Torsion angles [°] for ZC171-1abs

O(1)-C(1)-C(2)-C(7)	175.3(3)
C(17)-C(1)-C(2)-C(7)	-7.1(3)
O(1)-C(1)-C(2)-C(3)	-5.5(5)
C(17)-C(1)-C(2)-C(3)	172.2(3)
C(24)-O(3)-C(3)-C(4)	75.4(3)
C(24)-O(3)-C(3)-C(2)	-104.8(3)
C(7)-C(2)-C(3)-O(3)	-179.5(2)
C(1)-C(2)-C(3)-O(3)	1.4(4)
C(7)-C(2)-C(3)-C(4)	0.4(4)
C(1)-C(2)-C(3)-C(4)	-178.7(3)
C(25)-O(4)-C(4)-C(3)	82.9(3)
C(25)-O(4)-C(4)-C(5)	-99.1(3)
O(3)-C(3)-C(4)-O(4)	1.5(4)
C(2)-C(3)-C(4)-O(4)	-178.3(3)
O(3)-C(3)-C(4)-C(5)	-176.4(3)
C(2)-C(3)-C(4)-C(5)	3.7(4)
C(26)-O(5)-C(5)-C(6)	11.3(4)
C(26)-O(5)-C(5)-C(4)	-171.0(3)
O(4)-C(4)-C(5)-O(5)	-0.3(4)
C(3)-C(4)-C(5)-O(5)	177.7(3)
O(4)-C(4)-C(5)-C(6)	177.5(3)
C(3)-C(4)-C(5)-C(6)	-4.5(4)
O(5)-C(5)-C(6)-C(7)	178.7(2)
C(4)-C(5)-C(6)-C(7)	1.1(4)
C(5)-C(6)-C(7)-C(2)	3.0(4)
C(5)-C(6)-C(7)-C(8)	-175.3(2)
C(3)-C(2)-C(7)-C(6)	-3.8(4)
C(1)-C(2)-C(7)-C(6)	175.5(2)
C(3)-C(2)-C(7)-C(8)	174.7(2)
C(1)-C(2)-C(7)-C(8)	-6.0(3)
C(6)-C(7)-C(8)-C(9)	-38.6(3)
C(2)-C(7)-C(8)-C(9)	142.9(2)
C(6)-C(7)-C(8)-C(17)	-165.4(2)
C(2)-C(7)-C(8)-C(17)	16.1(3)
C(7)-C(8)-C(9)-C(14)	-93.2(3)
C(17)-C(8)-C(9)-C(14)	26.2(3)
C(7)-C(8)-C(9)-C(10)	84.0(3)
C(17)-C(8)-C(9)-C(10)	-156.6(2)
C(27)-O(6)-C(10)-C(11)	-44.7(4)
C(27)-O(6)-C(10)-C(9)	138.5(3)
C(14)-C(9)-C(10)-O(6)	175.0(2)
C(8)-C(9)-C(10)-O(6)	-2.2(4)

C(14)-C(9)-C(10)-C(11)	-1.9(4)
C(8)-C(9)-C(10)-C(11)	-179.1(2)
C(28)-O(7)-C(11)-C(10)	116.6(3)
C(28)-O(7)-C(11)-C(12)	-69.9(3)
O(6)-C(10)-C(11)-O(7)	1.8(4)
C(9)-C(10)-C(11)-O(7)	178.5(2)
O(6)-C(10)-C(11)-C(12)	-171.7(2)
C(9)-C(10)-C(11)-C(12)	4.9(4)
C(29)-O(8)-C(12)-C(13)	1.6(4)
C(29)-O(8)-C(12)-C(11)	-178.8(3)
O(7)-C(11)-C(12)-O(8)	2.5(4)
C(10)-C(11)-C(12)-O(8)	176.1(2)
O(7)-C(11)-C(12)-C(13)	-177.8(2)
C(10)-C(11)-C(12)-C(13)	-4.3(4)
O(8)-C(12)-C(13)-C(14)	-179.7(2)
C(11)-C(12)-C(13)-C(14)	0.6(4)
C(10)-C(9)-C(14)-C(13)	-1.8(4)
C(8)-C(9)-C(14)-C(13)	175.5(2)
C(10)-C(9)-C(14)-C(15)	173.3(2)
C(8)-C(9)-C(14)-C(15)	-9.4(3)
C(12)-C(13)-C(14)-C(9)	2.5(4)
C(12)-C(13)-C(14)-C(15)	-172.6(2)
C(9)-C(14)-C(15)-C(16)	-9.0(4)
C(13)-C(14)-C(15)-C(16)	166.2(2)
C(14)-C(15)-C(16)-C(17)	8.9(4)
C(14)-C(15)-C(16)-C(18)	-161.1(2)
C(15)-C(16)-C(17)-C(1)	124.8(2)
C(18)-C(16)-C(17)-C(1)	-65.3(3)
C(15)-C(16)-C(17)-C(8)	8.4(3)
C(18)-C(16)-C(17)-C(8)	178.3(2)
O(1)-C(1)-C(17)-C(16)	72.7(3)
C(2)-C(1)-C(17)-C(16)	-105.1(2)
O(1)-C(1)-C(17)-C(8)	-165.5(3)
C(2)-C(1)-C(17)-C(8)	16.7(3)
C(9)-C(8)-C(17)-C(16)	-24.9(3)
C(7)-C(8)-C(17)-C(16)	100.0(2)
C(9)-C(8)-C(17)-C(1)	-144.0(2)
C(7)-C(8)-C(17)-C(1)	-19.2(3)
C(15)-C(16)-C(18)-O(2)	97.1(3)
C(17)-C(16)-C(18)-O(2)	-73.3(3)
C(15)-C(16)-C(18)-N(19)	-76.7(3)
C(17)-C(16)-C(18)-N(19)	112.9(3)
O(2)-C(18)-N(19)-C(20)	163.4(2)
C(16)-C(18)-N(19)-C(20)	-23.1(4)

O(2)-C(18)-N(19)-C(23)	-0.7(4)
C(16)-C(18)-N(19)-C(23)	172.8(2)
C(18)-N(19)-C(20)-C(21)	-148.3(3)
C(23)-N(19)-C(20)-C(21)	17.2(4)
N(19)-C(20)-C(21)-C(22)	-19.5(5)
C(20)-C(21)-C(22)-C(23)	14.9(5)
C(18)-N(19)-C(23)-C(30)	-78.5(3)
C(20)-N(19)-C(23)-C(30)	115.3(3)
C(18)-N(19)-C(23)-C(22)	157.7(3)
C(20)-N(19)-C(23)-C(22)	-8.5(3)
C(21)-C(22)-C(23)-N(19)	-3.7(4)
C(21)-C(22)-C(23)-C(30)	-124.0(3)
N(19)-C(23)-C(30)-O(9)	-65.9(3)
C(22)-C(23)-C(30)-O(9)	50.2(3)

Table 7. Hydrogen bonds for ZC171-1abs [Å and °]

D-H····A	d(D-H)	d(H····A)	d(D····A)	<(DHA)
O(9)-H(9)···O(2)#1	0.96(4)	2.05(4)	2.923(3)	151(3)

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