A Catalytic Enantioselective Tandem Allylation Strategy for Rapid Terpene Construction: Application to the Synthesis of Pumilaside Aglycon

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Supporting Information - X-ray Crystallographic Data

Table of Contents

(1*R*,2*S*,3*S*,4*S*)-2-methyl-2-(4-methylpent-3-en-1-yl)-3-vinylcyclohexane-1,4-diol. (6) *S-2a*

(1*S*,2*S*,3*S*,4*R*)-2-methyl-2-(4-methylpent-3-en-1-yl)-3-vinyl-1,2,3,4-tetrahydronaphthalen

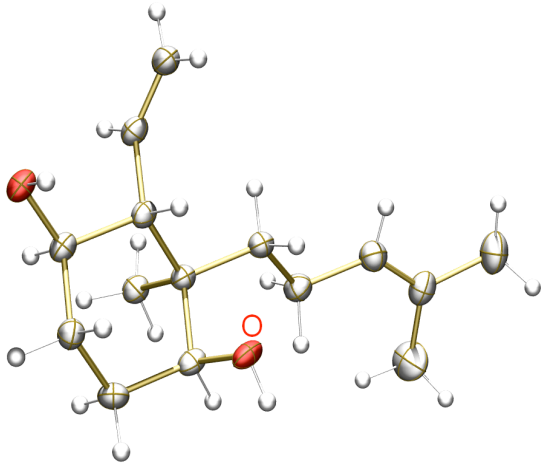
e-1,4-diol (4b) *S-13a*

(1*S*,2*R*,3*S*,4*R*)-2-methyl-2-(4-methylpent-3-en-1-yl)-3-vinyl-1,2,3,4-tetrahydronaphthalen

e-1,4-diol (*syn* diastereomer of 4c) *S-25a*

(1*R*,4*S*,5*S*)-5-vinylspiro[5.5]undecane-1,4-diol (4f) *S-45a*

(1R,2S,3S,4S)-2-methyl-2-(4-methylpent-3-en-1-yl)-3-vinylcyclohexane-1,4-diol. (6)



(*S,S*)-di-*iso*-propylTADDOL-PPh used when this crystal was obtained

Table 1. Crystal data and structure refinement for C15H26O2.

Identification code	C15H26O2	
Empirical formula	C15 H26 O2	
Formula weight	238.36	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 6.7212(6) Å	α= 90°.
	b = 7.0056(7) Å	β= 93.239(4)°.
	c = 15.1193(14) Å	γ = 90°.
Volume	710.77(12) $Å^3$	
Z	2	
Density (calculated)	1.114 Mg/m^3	
Absorption coefficient	0.555 mm^{-1}	
F(000)	264	
Crystal size	0.40 x 0.10 x 0.08 mm^3	
Theta range for data collection	2.93 to 66.49°.	
Index ranges	-7<=h<=7, -7<=k<=8, -17<=l<=17	
Reflections collected	8331	
Independent reflections	2356 [R(int) = 0.0250]	
Completeness to theta = 66.49°	97.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9569 and 0.8084	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2356 / 3 / 161
Goodness-of-fit on F^2	1.085
Final R indices [I>2sigma(I)]	R1 = 0.0312, wR2 = 0.0827
R indices (all data)	R1 = 0.0314, wR2 = 0.0829
Absolute structure parameter	0.03(17)
Extinction coefficient	na
Largest diff. peak and hole	0.183 and -0.158 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for C15H26O2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4634(1)	10492(1)	5998(1)	25(1)
O(2)	3420(1)	4128(1)	5450(1)	25(1)
C(1)	3401(2)	9678(2)	6646(1)	22(1)
C(2)	1480(2)	8911(2)	6194(1)	25(1)
C(3)	1889(2)	7263(2)	5565(1)	24(1)
C(4)	3057(2)	5676(2)	6042(1)	23(1)
C(5)	5010(2)	6447(2)	6496(1)	21(1)
C(6)	4599(2)	8098(2)	7155(1)	21(1)
C(7)	6202(2)	4839(2)	6919(1)	24(1)
C(8)	7966(2)	4278(2)	6681(1)	28(1)
C(9)	6606(2)	8893(2)	7536(1)	23(1)
C(10)	6528(2)	10279(2)	8311(1)	27(1)
C(11)	8563(2)	11104(2)	8558(1)	30(1)
C(12)	8979(2)	12613(2)	9063(1)	30(1)
C(13)	11069(3)	13319(3)	9240(1)	42(1)
C(14)	7410(3)	13756(3)	9492(1)	48(1)
C(15)	3374(2)	7387(2)	7921(1)	25(1)

Table 3. Bond lengths [Å] and angles [°] for C15H26O2.

O(1)-C(1)	1.4368(16)
O(1)-H(1O)	0.815(16)
O(2)-C(4)	1.4358(16)
O(2)-H(2O)	0.830(15)
C(1)-C(2)	1.5237(18)
C(1)-C(6)	1.5475(17)
C(1)-H(1)	1.0000
C(2)-C(3)	1.5298(19)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.5193(18)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.5448(17)
C(4)-H(4)	1.0000
C(5)-C(7)	1.5038(18)
C(5)-C(6)	1.5611(17)
C(5)-H(5)	1.0000
C(6)-C(9)	1.5401(17)
C(6)-C(15)	1.5412(17)
C(7)-C(8)	1.318(2)
C(7)-H(7)	0.9500
C(8)-H(8A)	0.9500
C(8)-H(8B)	0.9500
C(9)-C(10)	1.5256(19)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.5119(19)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.325(2)
C(11)-H(11)	0.9500
C(12)-C(13)	1.499(2)
C(12)-C(14)	1.500(2)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800

C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800

C(1)-O(1)-H(1O)	109.1(14)
C(4)-O(2)-H(2O)	108.0(14)
O(1)-C(1)-C(2)	109.93(10)
O(1)-C(1)-C(6)	108.61(10)
C(2)-C(1)-C(6)	112.01(11)
O(1)-C(1)-H(1)	108.7
C(2)-C(1)-H(1)	108.7
C(6)-C(1)-H(1)	108.7
C(1)-C(2)-C(3)	111.54(10)
C(1)-C(2)-H(2A)	109.3
C(3)-C(2)-H(2A)	109.3
C(1)-C(2)-H(2B)	109.3
C(3)-C(2)-H(2B)	109.3
H(2A)-C(2)-H(2B)	108.0
C(4)-C(3)-C(2)	111.32(10)
C(4)-C(3)-H(3A)	109.4
C(2)-C(3)-H(3A)	109.4
C(4)-C(3)-H(3B)	109.4
C(2)-C(3)-H(3B)	109.4
H(3A)-C(3)-H(3B)	108.0
O(2)-C(4)-C(3)	110.99(10)
O(2)-C(4)-C(5)	111.80(10)
C(3)-C(4)-C(5)	110.97(10)
O(2)-C(4)-H(4)	107.6
C(3)-C(4)-H(4)	107.6
C(5)-C(4)-H(4)	107.6
C(7)-C(5)-C(4)	110.23(11)
C(7)-C(5)-C(6)	113.14(10)
C(4)-C(5)-C(6)	111.48(10)
C(7)-C(5)-H(5)	107.2

C(4)-C(5)-H(5)	107.2
C(6)-C(5)-H(5)	107.2
C(9)-C(6)-C(15)	109.22(10)
C(9)-C(6)-C(1)	110.36(10)
C(15)-C(6)-C(1)	108.64(10)
C(9)-C(6)-C(5)	108.87(10)
C(15)-C(6)-C(5)	111.18(11)
C(1)-C(6)-C(5)	108.57(10)
C(8)-C(7)-C(5)	124.97(13)
C(8)-C(7)-H(7)	117.5
C(5)-C(7)-H(7)	117.5
C(7)-C(8)-H(8A)	120.0
C(7)-C(8)-H(8B)	120.0
H(8A)-C(8)-H(8B)	120.0
C(10)-C(9)-C(6)	116.76(11)
C(10)-C(9)-H(9A)	108.1
C(6)-C(9)-H(9A)	108.1
C(10)-C(9)-H(9B)	108.1
C(6)-C(9)-H(9B)	108.1
H(9A)-C(9)-H(9B)	107.3
C(11)-C(10)-C(9)	111.32(11)
C(11)-C(10)-H(10A)	109.4
C(9)-C(10)-H(10A)	109.4
C(11)-C(10)-H(10B)	109.4
C(9)-C(10)-H(10B)	109.4
H(10A)-C(10)-H(10B)	108.0
C(12)-C(11)-C(10)	127.32(13)
C(12)-C(11)-H(11)	116.3
C(10)-C(11)-H(11)	116.3
C(11)-C(12)-C(13)	122.09(15)
C(11)-C(12)-C(14)	122.96(14)
C(13)-C(12)-C(14)	114.94(14)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5

C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(6)-C(15)-H(15A)	109.5
C(6)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(6)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C15H26O2. 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)	34(1)	15(1)	27(1)	3(1)	7(1)	2(1)
O(2)	32(1)	18(1)	24(1)	-1(1)	3(1)	-2(1)
C(1)	28(1)	18(1)	22(1)	-1(1)	5(1)	2(1)
C(2)	25(1)	24(1)	26(1)	2(1)	0(1)	5(1)
C(3)	25(1)	22(1)	24(1)	0(1)	0(1)	-2(1)
C(4)	27(1)	18(1)	23(1)	0(1)	2(1)	-1(1)
C(5)	23(1)	18(1)	22(1)	2(1)	4(1)	-1(1)
C(6)	22(1)	18(1)	22(1)	0(1)	1(1)	1(1)
C(7)	30(1)	18(1)	24(1)	3(1)	1(1)	0(1)
C(8)	27(1)	22(1)	34(1)	-1(1)	-3(1)	1(1)
C(9)	24(1)	20(1)	26(1)	0(1)	0(1)	1(1)
C(10)	29(1)	25(1)	26(1)	-1(1)	0(1)	1(1)
C(11)	30(1)	29(1)	30(1)	-1(1)	0(1)	0(1)
C(12)	39(1)	28(1)	22(1)	3(1)	-3(1)	-6(1)
C(13)	47(1)	41(1)	37(1)	-3(1)	-2(1)	-15(1)
C(14)	52(1)	48(1)	45(1)	-22(1)	-4(1)	-2(1)
C(15)	28(1)	23(1)	23(1)	1(1)	2(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for C15H26O2.

	x	y	z	U(eq)
H(1O)	4240(30)	11570(20)	5877(12)	38
H(2O)	3990(20)	4570(30)	5021(10)	37
H(1)	3057	10697	7074	27
H(2A)	792	9952	5856	30
H(2B)	588	8463	6650	30
H(3A)	608	6749	5312	29
H(3B)	2654	7744	5071	29
H(4)	2221	5172	6516	27
H(5)	5816	6995	6021	25
H(7)	5641	4178	7394	29
H(8A)	8576	4905	6210	33
H(8B)	8627	3247	6982	33
H(9A)	7458	7800	7728	28
H(9B)	7268	9545	7051	28
H(10A)	5590	11329	8149	32
H(10B)	6025	9605	8829	32
H(11)	9667	10469	8325	36
H(13A)	11992	12489	8939	63
H(13B)	11406	13303	9879	63
H(13C)	11177	14626	9016	63
H(14A)	6098	13194	9345	73
H(14B)	7433	15074	9275	73
H(14C)	7675	13748	10136	73
H(15A)	4208	6563	8312	37
H(15B)	2219	6664	7680	37
H(15C)	2918	8483	8257	37

Table 6. Torsion angles [°] for C15H26O2.

O(1)-C(1)-C(2)-C(3)	64.25(14)
C(6)-C(1)-C(2)-C(3)	-56.60(14)
C(1)-C(2)-C(3)-C(4)	55.59(14)
C(2)-C(3)-C(4)-O(2)	179.50(10)
C(2)-C(3)-C(4)-C(5)	-55.54(14)
O(2)-C(4)-C(5)-C(7)	-52.21(13)
C(3)-C(4)-C(5)-C(7)	-176.71(10)
O(2)-C(4)-C(5)-C(6)	-178.72(10)
C(3)-C(4)-C(5)-C(6)	56.78(13)
O(1)-C(1)-C(6)-C(9)	53.70(13)
C(2)-C(1)-C(6)-C(9)	175.31(10)
O(1)-C(1)-C(6)-C(15)	173.42(10)
C(2)-C(1)-C(6)-C(15)	-64.97(13)
O(1)-C(1)-C(6)-C(5)	-65.54(12)
C(2)-C(1)-C(6)-C(5)	56.06(13)
C(7)-C(5)-C(6)-C(9)	58.89(14)
C(4)-C(5)-C(6)-C(9)	-176.21(10)
C(7)-C(5)-C(6)-C(15)	-61.47(14)
C(4)-C(5)-C(6)-C(15)	63.43(13)
C(7)-C(5)-C(6)-C(1)	179.07(11)
C(4)-C(5)-C(6)-C(1)	-56.03(13)
C(4)-C(5)-C(7)-C(8)	115.54(14)
C(6)-C(5)-C(7)-C(8)	-118.89(14)
C(15)-C(6)-C(9)-C(10)	-48.13(15)
C(1)-C(6)-C(9)-C(10)	71.25(14)
C(5)-C(6)-C(9)-C(10)	-169.69(11)
C(6)-C(9)-C(10)-C(11)	-174.11(12)
C(9)-C(10)-C(11)-C(12)	164.92(14)
C(10)-C(11)-C(12)-C(13)	-178.37(14)
C(10)-C(11)-C(12)-C(14)	0.9(2)

Symmetry transformations used to generate equivalent atoms:

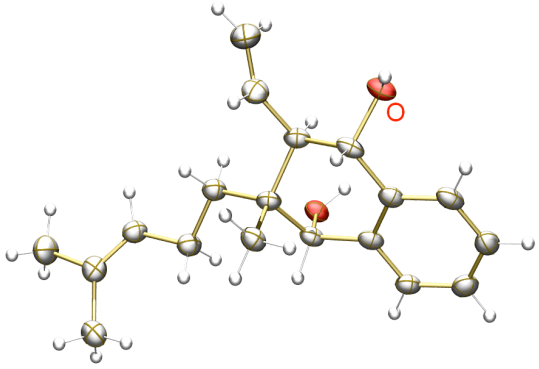
Table 7. Hydrogen bonds for C15H26O2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...O(2)#1	0.815(16)	1.976(16)	2.7863(13)	173.3(19)
O(2)-H(2O)...O(1)#2	0.830(15)	1.952(15)	2.7817(13)	177.5(19)

Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z #2 -x+1,y-1/2,-z+1

(1S,2S,3S,4R)-2-methyl-2-(4-methylpent-3-en-1-yl)-3-vinyl-1,2,3,4-tetrahydronaphthalene-1,4-diol (4b)



(*S,S*)-di-*iso*-propylTADDOL-PPh used when this crystal was obtained

Table 1. Crystal data and structure refinement for sad.

Identification code	C19H26O2	
Empirical formula	C19 H26 O2	
Formula weight	286.40	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 8.5973(10) Å	α= 90°.
	b = 7.2630(10) Å	β= 91.863(9)°.
	c = 13.3032(16) Å	γ = 90°.
Volume	830.24(18) $Å^3$	
Z	2	
Density (calculated)	1.146 Mg/m^3	
Absorption coefficient	0.562 mm^{-1}	
F(000)	312	
Crystal size	0.15 x 0.05 x 0.04 mm^3	
Theta range for data collection	3.32 to 65.43°.	
Index ranges	-10<=h<=10, -7<=k<=8, -15<=l<=15	
Reflections collected	9045	
Independent reflections	2711 [R(int) = 0.0593]	
Completeness to theta = 65.43°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9779 and 0.9204	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2711 / 6 / 208	

Goodness-of-fit on F^2	1.080
Final R indices [I>2sigma(I)]	R1 = 0.0473, wR2 = 0.1116
R indices (all data)	R1 = 0.0561, wR2 = 0.1159
Extinction coefficient	0.0102(17)
Largest diff. peak and hole	0.199 and -0.163 e.$Å^{-3}$
Absolute structure parameter	-0.2(3)

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

	x	y	z	U(eq)
O(1)	8633(2)	2367(3)	9130(1)	29(1)
O(2)	9449(2)	8730(3)	9372(1)	32(1)
C(1)	7340(3)	3568(4)	8893(2)	27(1)
C(2)	7023(2)	4739(4)	9807(2)	27(1)
C(3)	6308(3)	3892(4)	10625(2)	30(1)
C(4)	6139(3)	4853(4)	11512(2)	35(1)
C(5)	6666(3)	6629(4)	11603(2)	33(1)
C(6)	7331(3)	7492(4)	10793(2)	33(1)
C(7)	7515(2)	6546(4)	9890(2)	27(1)
C(8)	8234(3)	7521(4)	9011(2)	28(1)
C(9)	8879(3)	6189(4)	8242(2)	28(1)
C(10)	7633(2)	4717(4)	7950(2)	27(1)
C(11)	9494(3)	7204(4)	7356(2)	36(1)
C(12)	10970(4)	7305(6)	7135(2)	52(1)
C(13)	8229(3)	3484(4)	7099(2)	30(1)
C(14)	7261(3)	1776(4)	6860(2)	32(1)
C(15)	7795(3)	781(4)	5938(2)	33(1)
C(16)	6952(3)	-297(4)	5321(2)	34(1)
C(17)	5239(3)	-664(5)	5420(2)	40(1)
C(18)	7679(4)	-1300(5)	4464(2)	49(1)
C(19)	6090(3)	5621(4)	7597(2)	32(1)

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

O(1)-C(1)	1.440(3)
O(1)-H(1O)	0.845(18)
O(2)-C(8)	1.435(3)
O(2)-H(2O)	0.897(18)
C(1)-C(2)	1.515(4)
C(1)-C(10)	1.535(4)
C(1)-H(1)	1.002(17)
C(2)-C(7)	1.382(4)
C(2)-C(3)	1.409(4)
C(3)-C(4)	1.383(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.371(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.386(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.398(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.516(4)
C(8)-C(9)	1.526(4)
C(8)-H(8)	1.028(17)
C(9)-C(11)	1.502(4)
C(9)-C(10)	1.554(3)
C(9)-H(9)	1.011(17)
C(10)-C(19)	1.539(3)
C(10)-C(13)	1.544(4)
C(11)-C(12)	1.313(4)
C(11)-H(11)	0.9500
C(12)-H(12A)	0.9500
C(12)-H(12B)	0.9500
C(13)-C(14)	1.522(4)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.508(4)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.332(4)

C(15)-H(15A)	0.9500
C(16)-C(18)	1.506(4)
C(16)-C(17)	1.506(4)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800

C(1)-O(1)-H(1O)	107(2)
C(8)-O(2)-H(2O)	111(2)
O(1)-C(1)-C(2)	108.76(18)
O(1)-C(1)-C(10)	111.26(19)
C(2)-C(1)-C(10)	112.9(2)
O(1)-C(1)-H(1)	103.0(16)
C(2)-C(1)-H(1)	109.7(15)
C(10)-C(1)-H(1)	110.8(15)
C(7)-C(2)-C(3)	119.5(2)
C(7)-C(2)-C(1)	122.3(2)
C(3)-C(2)-C(1)	118.0(2)
C(4)-C(3)-C(2)	120.0(3)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(5)-C(4)-C(3)	120.4(3)
C(5)-C(4)-H(4)	119.8
C(3)-C(4)-H(4)	119.8
C(4)-C(5)-C(6)	120.0(3)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(7)	120.5(3)
C(5)-C(6)-H(6)	119.8
C(7)-C(6)-H(6)	119.8
C(2)-C(7)-C(6)	119.5(2)
C(2)-C(7)-C(8)	120.9(2)

C(6)-C(7)-C(8)	119.6(2)
O(2)-C(8)-C(7)	109.78(19)
O(2)-C(8)-C(9)	109.61(19)
C(7)-C(8)-C(9)	112.8(2)
O(2)-C(8)-H(8)	104.6(17)
C(7)-C(8)-H(8)	110.7(15)
C(9)-C(8)-H(8)	109.0(15)
C(11)-C(9)-C(8)	111.1(2)
C(11)-C(9)-C(10)	113.5(2)
C(8)-C(9)-C(10)	109.96(19)
C(11)-C(9)-H(9)	109.1(16)
C(8)-C(9)-H(9)	107.7(16)
C(10)-C(9)-H(9)	105.1(18)
C(1)-C(10)-C(19)	108.59(19)
C(1)-C(10)-C(13)	110.6(2)
C(19)-C(10)-C(13)	109.1(2)
C(1)-C(10)-C(9)	107.4(2)
C(19)-C(10)-C(9)	111.3(2)
C(13)-C(10)-C(9)	109.85(19)
C(12)-C(11)-C(9)	124.8(3)
C(12)-C(11)-H(11)	117.6
C(9)-C(11)-H(11)	117.6
C(11)-C(12)-H(12A)	120.0
C(11)-C(12)-H(12B)	120.0
H(12A)-C(12)-H(12B)	120.0
C(14)-C(13)-C(10)	115.69(19)
C(14)-C(13)-H(13A)	108.4
C(10)-C(13)-H(13A)	108.4
C(14)-C(13)-H(13B)	108.4
C(10)-C(13)-H(13B)	108.4
H(13A)-C(13)-H(13B)	107.4
C(15)-C(14)-C(13)	112.4(2)
C(15)-C(14)-H(14A)	109.1
C(13)-C(14)-H(14A)	109.1
C(15)-C(14)-H(14B)	109.1
C(13)-C(14)-H(14B)	109.1
H(14A)-C(14)-H(14B)	107.8
C(16)-C(15)-C(14)	127.5(2)

C(16)-C(15)-H(15A)	116.2
C(14)-C(15)-H(15A)	116.2
C(15)-C(16)-C(18)	121.3(2)
C(15)-C(16)-C(17)	124.3(2)
C(18)-C(16)-C(17)	114.3(2)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(10)-C(19)-H(19A)	109.5
C(10)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(10)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sad. 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)	22(1)	26(1)	39(1)	-4(1)	-3(1)	2(1)
O(2)	27(1)	23(1)	47(1)	1(1)	-6(1)	-3(1)
C(1)	19(1)	23(2)	38(1)	-3(1)	-1(1)	0(1)
C(2)	14(1)	27(2)	39(1)	0(1)	-2(1)	4(1)
C(3)	20(1)	30(2)	40(2)	-1(1)	2(1)	-1(1)
C(4)	21(1)	44(2)	40(2)	1(1)	5(1)	2(1)
C(5)	22(1)	38(2)	39(2)	-8(1)	2(1)	4(1)
C(6)	19(1)	30(2)	48(2)	-9(1)	-3(1)	0(1)
C(7)	15(1)	29(2)	37(1)	-1(1)	-3(1)	4(1)
C(8)	19(1)	21(2)	44(2)	-1(1)	-6(1)	-1(1)
C(9)	20(1)	25(2)	39(1)	3(1)	1(1)	0(1)
C(10)	18(1)	28(2)	36(1)	2(1)	0(1)	-1(1)
C(11)	40(2)	26(2)	42(2)	0(1)	3(1)	-7(1)
C(12)	49(2)	57(2)	49(2)	1(2)	10(1)	-20(2)
C(13)	24(1)	30(2)	36(1)	-1(1)	2(1)	-1(1)
C(14)	28(1)	31(2)	39(2)	-5(1)	4(1)	-2(1)
C(15)	28(1)	32(2)	39(1)	-2(1)	6(1)	0(1)
C(16)	37(1)	28(2)	38(2)	0(1)	2(1)	3(1)
C(17)	39(1)	39(2)	41(2)	0(1)	-5(1)	-2(1)
C(18)	51(2)	51(2)	47(2)	-18(2)	8(1)	-5(2)
C(19)	26(1)	32(2)	37(1)	-3(1)	-3(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for sad.

	x	y	z	U(eq)
H(1O)	9200(30)	2900(40)	9573(19)	44
H(2O)	9200(40)	9910(30)	9250(20)	48
H(1)	6460(30)	2690(30)	8768(19)	32
H(3)	5941	2661	10567	36
H(4)	5655	4279	12062	42
H(5)	6576	7268	12222	40
H(6)	7665	8736	10853	39
H(8)	7440(30)	8370(40)	8656(18)	34
H(9)	9760(30)	5480(40)	8585(18)	33
H(11)	8763	7818	6923	43
H(12A)	11735	6708	7550	62
H(12B)	11272	7974	6559	62
H(13A)	8281	4236	6480	36
H(13B)	9303	3089	7284	36
H(14A)	7325	927	7442	39
H(14B)	6158	2139	6754	39
H(15A)	8855	942	5779	39
H(17A)	5080	-1965	5583	59
H(17B)	4687	-371	4784	59
H(17C)	4835	106	5958	59
H(18A)	8799	-1042	4470	74
H(18B)	7200	-884	3826	74
H(18C)	7514	-2627	4539	74
H(19A)	5330	4662	7415	48
H(19B)	6269	6399	7010	48
H(19C)	5690	6377	8141	48

Table 6. Torsion angles [°] for sad.

O(1)-C(1)-C(2)-C(7)	101.1(3)
C(10)-C(1)-C(2)-C(7)	-22.9(3)
O(1)-C(1)-C(2)-C(3)	-74.0(3)
C(10)-C(1)-C(2)-C(3)	162.04(19)
C(7)-C(2)-C(3)-C(4)	-1.7(3)
C(1)-C(2)-C(3)-C(4)	173.5(2)
C(2)-C(3)-C(4)-C(5)	-0.1(3)
C(3)-C(4)-C(5)-C(6)	1.9(4)
C(4)-C(5)-C(6)-C(7)	-2.0(4)
C(3)-C(2)-C(7)-C(6)	1.7(3)
C(1)-C(2)-C(7)-C(6)	-173.3(2)
C(3)-C(2)-C(7)-C(8)	-177.7(2)
C(1)-C(2)-C(7)-C(8)	7.3(3)
C(5)-C(6)-C(7)-C(2)	0.2(3)
C(5)-C(6)-C(7)-C(8)	179.5(2)
C(2)-C(7)-C(8)-O(2)	-143.7(2)
C(6)-C(7)-C(8)-O(2)	36.9(3)
C(2)-C(7)-C(8)-C(9)	-21.2(3)
C(6)-C(7)-C(8)-C(9)	159.46(19)
O(2)-C(8)-C(9)-C(11)	-60.7(3)
C(7)-C(8)-C(9)-C(11)	176.65(19)
O(2)-C(8)-C(9)-C(10)	172.7(2)
C(7)-C(8)-C(9)-C(10)	50.1(3)
O(1)-C(1)-C(10)-C(19)	167.0(2)
C(2)-C(1)-C(10)-C(19)	-70.3(3)
O(1)-C(1)-C(10)-C(13)	47.4(3)
C(2)-C(1)-C(10)-C(13)	170.03(18)
O(1)-C(1)-C(10)-C(9)	-72.5(2)
C(2)-C(1)-C(10)-C(9)	50.2(2)
C(11)-C(9)-C(10)-C(1)	169.8(2)
C(8)-C(9)-C(10)-C(1)	-65.0(2)
C(11)-C(9)-C(10)-C(19)	-71.4(3)
C(8)-C(9)-C(10)-C(19)	53.7(3)
C(11)-C(9)-C(10)-C(13)	49.5(3)
C(8)-C(9)-C(10)-C(13)	174.6(2)
C(8)-C(9)-C(11)-C(12)	111.8(3)

C(10)-C(9)-C(11)-C(12)	-123.7(3)
C(1)-C(10)-C(13)-C(14)	51.3(3)
C(19)-C(10)-C(13)-C(14)	-68.1(3)
C(9)-C(10)-C(13)-C(14)	169.7(2)
C(10)-C(13)-C(14)-C(15)	172.6(2)
C(13)-C(14)-C(15)-C(16)	-154.0(3)
C(14)-C(15)-C(16)-C(18)	-175.9(3)
C(14)-C(15)-C(16)-C(17)	2.5(5)

Symmetry transformations used to generate equivalent atoms:

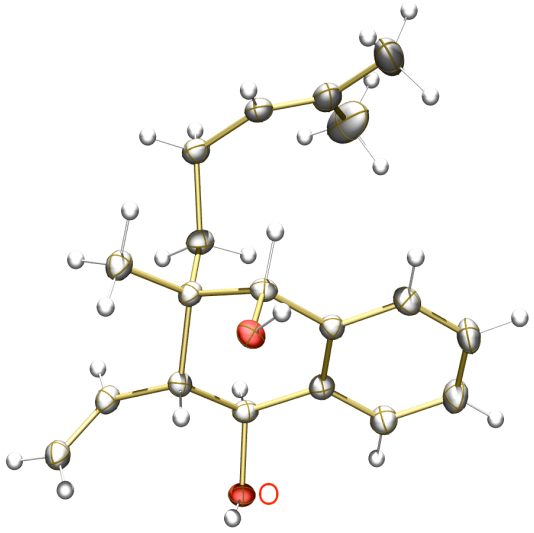
Table 7. Hydrogen bonds for sad [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...O(2)#1	0.845(18)	1.892(18)	2.730(2)	171(3)
O(2)-H(2O)...O(1)#2	0.897(18)	1.855(19)	2.749(3)	175(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y-1/2,-z+2 #2 x,y+1,z

(1S,2R,3S,4R)-2-methyl-2-(4-methylpent-3-en-1-yl)-3-vinyl-1,2,3,4-tetrahydronaphthalene-1,4-diol (syn diastereomer of 4c)



(*S,S*)-di-*iso*-propylTADDOL-PPh used when this crystal was obtained

Table 1. Crystal data and structure refinement for C19H26O2.

Identification code	C19H26O2	
Empirical formula	C19 H26 O2	
Formula weight	286.40	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 14.6441(14) Å	α= 90°.
	b = 6.9021(7) Å	β= 106.762(4)°.
	c = 16.9049(16) Å	γ = 90°.
Volume	1636.1(3) $Å^3$	
Z	4	
Density (calculated)	1.163 Mg/m^3	
Absorption coefficient	0.570 mm^{-1}	
F(000)	624	
Crystal size	0.12 x 0.08 x 0.04 mm^3	
Theta range for data collection	2.73 to 67.34°.	
Index ranges	-17<=h<=17, -4<=k<=8, -20<=l<=20	
Reflections collected	14863	
Independent reflections	3901 [R(int) = 0.0422]	
Completeness to theta = 67.34°	97.8 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.9775 and 0.9347
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3901 / 11 / 415
Goodness-of-fit on F^2	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0337, wR2 = 0.0878
R indices (all data)	R1 = 0.0347, wR2 = 0.0888
Absolute structure parameter	0.34(18)
Extinction coefficient	na
Largest diff. peak and hole	0.175 and -0.225 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for C19H26O2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	575(1)	2164(2)	4541(1)	20(1)
O(2)	1110(1)	-4177(2)	5205(1)	20(1)
C(1)	1392(1)	1415(3)	4324(1)	18(1)
C(2)	1058(1)	-123(3)	3646(1)	19(1)
C(3)	687(1)	-1875(3)	4050(1)	18(1)
C(4)	1487(1)	-2788(3)	4746(1)	19(1)
C(5)	2118(1)	-1313(3)	5315(1)	19(1)
C(6)	2757(1)	-1936(3)	6058(1)	26(1)
C(7)	3378(1)	-646(4)	6568(1)	31(1)
C(8)	3379(1)	1300(3)	6342(1)	30(1)
C(9)	2748(1)	1922(3)	5612(1)	24(1)
C(10)	2108(1)	638(3)	5094(1)	19(1)
C(11)	243(1)	694(3)	2941(1)	25(1)
C(12)	1902(1)	-773(3)	3322(1)	23(1)
C(13)	2240(1)	637(3)	2758(1)	25(1)
C(14)	2695(1)	2489(3)	3153(1)	26(1)
C(15)	3577(2)	2696(4)	3651(1)	38(1)
C(16)	4270(2)	1056(7)	3885(2)	68(1)
C(17)	3908(2)	4658(6)	4033(2)	62(1)
C(18)	190(1)	-3397(3)	3443(1)	22(1)
C(19)	-685(1)	-4009(3)	3358(1)	27(1)
O(3)	5619(1)	2396(2)	9546(1)	19(1)
O(4)	5988(1)	-4101(2)	10248(1)	20(1)
C(20)	6553(1)	1621(3)	9636(1)	18(1)
C(21)	6488(1)	97(3)	8958(1)	18(1)
C(22)	5970(1)	-1705(3)	9172(1)	18(1)
C(23)	6528(1)	-2615(3)	10000(1)	18(1)
C(24)	6886(1)	-1136(3)	10685(1)	18(1)
C(25)	7193(1)	-1754(3)	11508(1)	21(1)
C(26)	7575(1)	-462(3)	12140(1)	24(1)
C(27)	7663(1)	1485(3)	11961(1)	24(1)
C(28)	7351(1)	2119(3)	11150(1)	21(1)

C(29)	6955(1)	832(3)	10506(1)	18(1)
C(30)	5899(1)	909(3)	8120(1)	21(1)
C(31)	7513(1)	-417(3)	8940(1)	19(1)
C(32)	8012(1)	1128(3)	8555(1)	22(1)
C(33)	9000(1)	490(3)	8579(1)	23(1)
C(34)	9818(1)	1430(4)	8891(1)	28(1)
C(35)	9908(2)	3408(4)	9276(1)	44(1)
C(36)	10750(1)	513(5)	8888(1)	40(1)
C(37)	5741(1)	-3219(3)	8503(1)	20(1)
C(38)	4893(1)	-3985(3)	8183(1)	24(1)

Table 3. Bond lengths [Å] and angles [°] for C19H26O2.

O(1)-C(1)	1.443(2)
O(1)-H(1O)	0.851(18)
O(2)-C(4)	1.440(2)
O(2)-H(2O)	0.860(17)
C(1)-C(10)	1.515(2)
C(1)-C(2)	1.535(3)
C(1)-H(1)	0.974(16)
C(2)-C(11)	1.532(2)
C(2)-C(12)	1.555(2)
C(2)-C(3)	1.562(3)
C(3)-C(18)	1.502(3)
C(3)-C(4)	1.536(2)
C(3)-H(3)	0.977(16)
C(4)-C(5)	1.518(3)
C(4)-H(4)	0.989(16)
C(5)-C(10)	1.396(3)
C(5)-C(6)	1.400(3)
C(6)-C(7)	1.383(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.397(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.379(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.398(3)
C(9)-H(9)	0.9500
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(13)	1.541(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.506(3)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.331(3)
C(14)-H(14)	0.9500

C(15)-C(16)	1.494(5)
C(15)-C(17)	1.519(4)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.317(3)
C(18)-H(18)	0.9500
C(19)-H(19A)	0.9500
C(19)-H(19B)	0.9500
O(3)-C(20)	1.436(2)
O(3)-H(3O)	0.822(18)
O(4)-C(23)	1.430(2)
O(4)-H(4O)	0.854(17)
C(20)-C(29)	1.519(2)
C(20)-C(21)	1.538(3)
C(20)-H(20)	1.005(16)
C(21)-C(30)	1.536(2)
C(21)-C(31)	1.551(2)
C(21)-C(22)	1.553(3)
C(22)-C(37)	1.505(3)
C(22)-C(23)	1.538(2)
C(22)-H(22)	0.991(15)
C(23)-C(24)	1.518(3)
C(23)-H(23)	1.004(16)
C(24)-C(25)	1.400(2)
C(24)-C(29)	1.402(3)
C(25)-C(26)	1.380(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.392(3)
C(26)-H(26)	0.9500
C(27)-C(28)	1.385(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.395(3)
C(28)-H(28)	0.9500
C(30)-H(30A)	0.9800

C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(32)	1.538(3)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(33)	1.503(2)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-C(34)	1.330(3)
C(33)-H(33)	0.9500
C(34)-C(35)	1.502(4)
C(34)-C(36)	1.507(3)
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(38)	1.314(3)
C(37)-H(37)	0.9500
C(38)-H(38A)	0.9500
C(38)-H(38B)	0.9500

C(1)-O(1)-H(1O)	108.8(17)
C(4)-O(2)-H(2O)	105.4(18)
O(1)-C(1)-C(10)	109.17(13)
O(1)-C(1)-C(2)	109.21(14)
C(10)-C(1)-C(2)	112.87(16)
O(1)-C(1)-H(1)	106.3(13)
C(10)-C(1)-H(1)	109.5(12)
C(2)-C(1)-H(1)	109.6(12)
C(11)-C(2)-C(1)	109.59(16)
C(11)-C(2)-C(12)	110.64(14)
C(1)-C(2)-C(12)	110.42(14)
C(11)-C(2)-C(3)	109.49(15)
C(1)-C(2)-C(3)	106.55(13)
C(12)-C(2)-C(3)	110.06(16)
C(18)-C(3)-C(4)	110.38(16)

C(18)-C(3)-C(2)	113.87(14)
C(4)-C(3)-C(2)	111.58(14)
C(18)-C(3)-H(3)	108.1(13)
C(4)-C(3)-H(3)	106.6(12)
C(2)-C(3)-H(3)	105.9(15)
O(2)-C(4)-C(5)	111.31(13)
O(2)-C(4)-C(3)	111.10(14)
C(5)-C(4)-C(3)	113.61(16)
O(2)-C(4)-H(4)	102.7(14)
C(5)-C(4)-H(4)	107.1(13)
C(3)-C(4)-H(4)	110.4(12)
C(10)-C(5)-C(6)	119.23(18)
C(10)-C(5)-C(4)	121.37(16)
C(6)-C(5)-C(4)	119.33(19)
C(7)-C(6)-C(5)	120.8(2)
C(7)-C(6)-H(6)	119.6
C(5)-C(6)-H(6)	119.6
C(6)-C(7)-C(8)	120.02(18)
C(6)-C(7)-H(7)	120.0
C(8)-C(7)-H(7)	120.0
C(9)-C(8)-C(7)	119.4(2)
C(9)-C(8)-H(8)	120.3
C(7)-C(8)-H(8)	120.3
C(8)-C(9)-C(10)	121.2(2)
C(8)-C(9)-H(9)	119.4
C(10)-C(9)-H(9)	119.4
C(5)-C(10)-C(9)	119.38(17)
C(5)-C(10)-C(1)	121.48(17)
C(9)-C(10)-C(1)	119.09(18)
C(2)-C(11)-H(11A)	109.5
C(2)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(2)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(13)-C(12)-C(2)	117.76(17)
C(13)-C(12)-H(12A)	107.9
C(2)-C(12)-H(12A)	107.9

C(13)-C(12)-H(12B)	107.9
C(2)-C(12)-H(12B)	107.9
H(12A)-C(12)-H(12B)	107.2
C(14)-C(13)-C(12)	116.17(15)
C(14)-C(13)-H(13A)	108.2
C(12)-C(13)-H(13A)	108.2
C(14)-C(13)-H(13B)	108.2
C(12)-C(13)-H(13B)	108.2
H(13A)-C(13)-H(13B)	107.4
C(15)-C(14)-C(13)	126.6(2)
C(15)-C(14)-H(14)	116.7
C(13)-C(14)-H(14)	116.7
C(14)-C(15)-C(16)	123.2(3)
C(14)-C(15)-C(17)	119.8(3)
C(16)-C(15)-C(17)	117.0(2)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-C(3)	124.29(17)
C(19)-C(18)-H(18)	117.9
C(3)-C(18)-H(18)	117.9
C(18)-C(19)-H(19A)	120.0
C(18)-C(19)-H(19B)	120.0
H(19A)-C(19)-H(19B)	120.0
C(20)-O(3)-H(3O)	106.3(17)
C(23)-O(4)-H(4O)	105.4(18)
O(3)-C(20)-C(29)	109.15(13)
O(3)-C(20)-C(21)	108.84(14)
C(29)-C(20)-C(21)	113.57(16)

O(3)-C(20)-H(20)	108.4(13)
C(29)-C(20)-H(20)	108.2(11)
C(21)-C(20)-H(20)	108.6(12)
C(30)-C(21)-C(20)	109.60(15)
C(30)-C(21)-C(31)	110.71(13)
C(20)-C(21)-C(31)	108.60(14)
C(30)-C(21)-C(22)	108.97(14)
C(20)-C(21)-C(22)	107.68(14)
C(31)-C(21)-C(22)	111.23(15)
C(37)-C(22)-C(23)	110.22(16)
C(37)-C(22)-C(21)	113.50(14)
C(23)-C(22)-C(21)	111.82(14)
C(37)-C(22)-H(22)	106.4(13)
C(23)-C(22)-H(22)	107.4(12)
C(21)-C(22)-H(22)	107.2(15)
O(4)-C(23)-C(24)	110.94(13)
O(4)-C(23)-C(22)	111.44(14)
C(24)-C(23)-C(22)	113.30(16)
O(4)-C(23)-H(23)	101.3(14)
C(24)-C(23)-H(23)	107.9(13)
C(22)-C(23)-H(23)	111.2(11)
C(25)-C(24)-C(29)	119.16(18)
C(25)-C(24)-C(23)	119.61(18)
C(29)-C(24)-C(23)	121.17(15)
C(26)-C(25)-C(24)	120.97(19)
C(26)-C(25)-H(25)	119.5
C(24)-C(25)-H(25)	119.5
C(25)-C(26)-C(27)	119.86(17)
C(25)-C(26)-H(26)	120.1
C(27)-C(26)-H(26)	120.1
C(28)-C(27)-C(26)	119.70(19)
C(28)-C(27)-H(27)	120.1
C(26)-C(27)-H(27)	120.1
C(27)-C(28)-C(29)	121.0(2)
C(27)-C(28)-H(28)	119.5
C(29)-C(28)-H(28)	119.5
C(28)-C(29)-C(24)	119.25(16)
C(28)-C(29)-C(20)	119.01(18)

C(24)-C(29)-C(20)	121.63(17)
C(21)-C(30)-H(30A)	109.5
C(21)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(21)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(21)	115.47(15)
C(32)-C(31)-H(31A)	108.4
C(21)-C(31)-H(31A)	108.4
C(32)-C(31)-H(31B)	108.4
C(21)-C(31)-H(31B)	108.4
H(31A)-C(31)-H(31B)	107.5
C(33)-C(32)-C(31)	110.92(16)
C(33)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32A)	109.5
C(33)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	108.0
C(34)-C(33)-C(32)	128.2(2)
C(34)-C(33)-H(33)	115.9
C(32)-C(33)-H(33)	115.9
C(33)-C(34)-C(35)	124.9(2)
C(33)-C(34)-C(36)	120.4(2)
C(35)-C(34)-C(36)	114.7(2)
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-C(22)	124.59(17)

C(38)-C(37)-H(37)	117.7
C(22)-C(37)-H(37)	117.7
C(37)-C(38)-H(38A)	120.0
C(37)-C(38)-H(38B)	120.0
H(38A)-C(38)-H(38B)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C19H26O2. 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)	22(1)	14(1)	26(1)	-2(1)	8(1)	1(1)
O(2)	24(1)	15(1)	23(1)	2(1)	9(1)	0(1)
C(1)	20(1)	14(1)	22(1)	2(1)	9(1)	1(1)
C(2)	22(1)	18(1)	17(1)	2(1)	5(1)	1(1)
C(3)	20(1)	16(1)	19(1)	-2(1)	7(1)	0(1)
C(4)	23(1)	15(1)	20(1)	1(1)	10(1)	0(1)
C(5)	20(1)	19(1)	20(1)	0(1)	8(1)	2(1)
C(6)	27(1)	23(1)	26(1)	2(1)	6(1)	1(1)
C(7)	28(1)	34(1)	25(1)	3(1)	-2(1)	1(1)
C(8)	28(1)	29(1)	28(1)	-6(1)	0(1)	-6(1)
C(9)	25(1)	18(1)	28(1)	-1(1)	8(1)	-2(1)
C(10)	20(1)	19(1)	20(1)	-1(1)	8(1)	-1(1)
C(11)	29(1)	22(1)	21(1)	1(1)	4(1)	0(1)
C(12)	29(1)	19(1)	22(1)	0(1)	11(1)	0(1)
C(13)	30(1)	27(1)	22(1)	0(1)	11(1)	-3(1)
C(14)	29(1)	28(1)	22(1)	2(1)	11(1)	-5(1)
C(15)	34(1)	58(2)	24(1)	2(1)	10(1)	-14(1)
C(16)	29(1)	120(3)	52(1)	30(2)	8(1)	9(2)
C(17)	60(2)	93(3)	35(1)	-18(1)	20(1)	-48(2)
C(18)	28(1)	18(1)	19(1)	-2(1)	6(1)	1(1)
C(19)	30(1)	24(1)	22(1)	0(1)	4(1)	-6(1)
O(3)	18(1)	15(1)	25(1)	-1(1)	7(1)	2(1)
O(4)	21(1)	15(1)	28(1)	0(1)	10(1)	-1(1)
C(20)	16(1)	15(1)	23(1)	1(1)	7(1)	0(1)
C(21)	17(1)	17(1)	19(1)	0(1)	6(1)	0(1)
C(22)	16(1)	16(1)	22(1)	-1(1)	7(1)	1(1)
C(23)	17(1)	15(1)	24(1)	0(1)	8(1)	-1(1)
C(24)	14(1)	19(1)	23(1)	0(1)	7(1)	1(1)
C(25)	19(1)	20(1)	24(1)	2(1)	6(1)	3(1)
C(26)	21(1)	30(1)	19(1)	2(1)	3(1)	4(1)
C(27)	19(1)	27(1)	24(1)	-7(1)	3(1)	-2(1)
C(28)	18(1)	18(1)	27(1)	-2(1)	6(1)	-1(1)
C(29)	14(1)	20(1)	21(1)	-2(1)	7(1)	0(1)

C(30)	19(1)	20(1)	22(1)	-1(1)	5(1)	1(1)
C(31)	19(1)	17(1)	20(1)	-1(1)	6(1)	0(1)
C(32)	24(1)	20(1)	24(1)	1(1)	9(1)	0(1)
C(33)	24(1)	26(1)	20(1)	0(1)	9(1)	0(1)
C(34)	25(1)	43(1)	17(1)	2(1)	6(1)	-7(1)
C(35)	41(1)	51(2)	37(1)	-13(1)	9(1)	-20(1)
C(36)	22(1)	64(2)	32(1)	1(1)	8(1)	-6(1)
C(37)	22(1)	16(1)	22(1)	-1(1)	6(1)	1(1)
C(38)	26(1)	20(1)	25(1)	-1(1)	4(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for C19H26O2.

	x	y	z	U(eq)
H(1O)	692(17)	3320(30)	4713(14)	30
H(2O)	618(13)	-3630(40)	5289(13)	31
H(1)	1669(14)	2510(30)	4111(12)	22
H(3)	226(13)	-1340(40)	4309(12)	22
H(4)	1905(14)	-3590(30)	4512(12)	23
H(6)	2763	-3259	6213	31
H(7)	3805	-1084	7073	37
H(8)	3810	2188	6688	36
H(9)	2747	3246	5458	29
H(11A)	-326	857	3130	37
H(11B)	100	-203	2472	37
H(11C)	431	1953	2769	37
H(12A)	2453	-1058	3807	27
H(12B)	1718	-2003	3017	27
H(13A)	2705	-51	2534	30
H(13B)	1685	975	2285	30
H(14)	2313	3624	3036	31
H(16A)	4026	-60	3528	101
H(16B)	4352	699	4462	101
H(16C)	4885	1455	3817	101
H(17A)	3416	5631	3802	92
H(17B)	4500	5024	3912	92
H(17C)	4022	4586	4633	92
H(18)	529	-3956	3098	26
H(19A)	-1044	-3480	3693	32
H(19B)	-957	-4979	2961	32
H(3O)	5698(17)	3500(30)	9738(14)	29
H(4O)	5496(13)	-3530(40)	10313(13)	31
H(20)	6977(13)	2700(30)	9558(12)	21
H(22)	5350(12)	-1250(40)	9231(12)	21
H(23)	7093(13)	-3370(30)	9945(12)	22
H(25)	7138	-3083	11634	26

H(26)	7777	-900	12696	29
H(27)	7937	2376	12393	28
H(28)	7406	3451	11030	26
H(30A)	5228	999	8109	31
H(30B)	5959	46	7677	31
H(30C)	6136	2200	8039	31
H(31A)	7909	-660	9513	22
H(31B)	7486	-1639	8627	22
H(32A)	7634	1361	7975	26
H(32B)	8047	2360	8863	26
H(33)	9047	-740	8341	27
H(35A)	9275	3999	9162	65
H(35B)	10315	4220	9043	65
H(35C)	10193	3295	9875	65
H(36A)	10630	-773	8633	59
H(36B)	11161	387	9456	59
H(36C)	11067	1327	8571	59
H(37)	6245	-3650	8297	24
H(38A)	4372	-3588	8374	29
H(38B)	4800	-4937	7761	29

Table 6. Torsion angles [°] for C19H26O2.

O(1)-C(1)-C(2)-C(11)	50.83(18)
C(10)-C(1)-C(2)-C(11)	172.46(15)
O(1)-C(1)-C(2)-C(12)	172.95(14)
C(10)-C(1)-C(2)-C(12)	-65.42(18)
O(1)-C(1)-C(2)-C(3)	-67.55(17)
C(10)-C(1)-C(2)-C(3)	54.08(18)
C(11)-C(2)-C(3)-C(18)	52.5(2)
C(1)-C(2)-C(3)-C(18)	170.97(14)
C(12)-C(2)-C(3)-C(18)	-69.29(18)
C(11)-C(2)-C(3)-C(4)	178.29(15)
C(1)-C(2)-C(3)-C(4)	-63.27(18)
C(12)-C(2)-C(3)-C(4)	56.47(18)
C(18)-C(3)-C(4)-O(2)	-62.15(18)
C(2)-C(3)-C(4)-O(2)	170.18(14)
C(18)-C(3)-C(4)-C(5)	171.42(14)
C(2)-C(3)-C(4)-C(5)	43.75(18)
O(2)-C(4)-C(5)-C(10)	-141.30(16)
C(3)-C(4)-C(5)-C(10)	-15.0(2)
O(2)-C(4)-C(5)-C(6)	41.8(2)
C(3)-C(4)-C(5)-C(6)	168.13(15)
C(10)-C(5)-C(6)-C(7)	-0.5(3)
C(4)-C(5)-C(6)-C(7)	176.45(17)
C(5)-C(6)-C(7)-C(8)	-0.5(3)
C(6)-C(7)-C(8)-C(9)	0.8(3)
C(7)-C(8)-C(9)-C(10)	-0.1(3)
C(6)-C(5)-C(10)-C(9)	1.2(3)
C(4)-C(5)-C(10)-C(9)	-175.72(15)
C(6)-C(5)-C(10)-C(1)	-176.16(15)
C(4)-C(5)-C(10)-C(1)	6.9(2)
C(8)-C(9)-C(10)-C(5)	-0.9(3)
C(8)-C(9)-C(10)-C(1)	176.50(16)
O(1)-C(1)-C(10)-C(5)	93.69(19)
C(2)-C(1)-C(10)-C(5)	-28.0(2)
O(1)-C(1)-C(10)-C(9)	-83.7(2)
C(2)-C(1)-C(10)-C(9)	154.70(16)
C(11)-C(2)-C(12)-C(13)	47.4(2)

C(1)-C(2)-C(12)-C(13)	-74.1(2)
C(3)-C(2)-C(12)-C(13)	168.50(15)
C(2)-C(12)-C(13)-C(14)	66.8(2)
C(12)-C(13)-C(14)-C(15)	77.3(2)
C(13)-C(14)-C(15)-C(16)	0.9(3)
C(13)-C(14)-C(15)-C(17)	-176.89(18)
C(4)-C(3)-C(18)-C(19)	109.5(2)
C(2)-C(3)-C(18)-C(19)	-124.1(2)
O(3)-C(20)-C(21)-C(30)	47.14(18)
C(29)-C(20)-C(21)-C(30)	168.94(14)
O(3)-C(20)-C(21)-C(31)	168.20(14)
C(29)-C(20)-C(21)-C(31)	-70.00(18)
O(3)-C(20)-C(21)-C(22)	-71.25(17)
C(29)-C(20)-C(21)-C(22)	50.55(18)
C(30)-C(21)-C(22)-C(37)	53.68(19)
C(20)-C(21)-C(22)-C(37)	172.49(14)
C(31)-C(21)-C(22)-C(37)	-68.64(18)
C(30)-C(21)-C(22)-C(23)	179.14(14)
C(20)-C(21)-C(22)-C(23)	-62.05(18)
C(31)-C(21)-C(22)-C(23)	56.82(18)
C(37)-C(22)-C(23)-O(4)	-60.79(18)
C(21)-C(22)-C(23)-O(4)	171.97(14)
C(37)-C(22)-C(23)-C(24)	173.25(14)
C(21)-C(22)-C(23)-C(24)	46.00(18)
O(4)-C(23)-C(24)-C(25)	38.0(2)
C(22)-C(23)-C(24)-C(25)	164.21(15)
O(4)-C(23)-C(24)-C(29)	-144.89(16)
C(22)-C(23)-C(24)-C(29)	-18.7(2)
C(29)-C(24)-C(25)-C(26)	-1.1(3)
C(23)-C(24)-C(25)-C(26)	176.09(15)
C(24)-C(25)-C(26)-C(27)	-0.4(3)
C(25)-C(26)-C(27)-C(28)	1.2(3)
C(26)-C(27)-C(28)-C(29)	-0.6(3)
C(27)-C(28)-C(29)-C(24)	-0.8(2)
C(27)-C(28)-C(29)-C(20)	175.34(15)
C(25)-C(24)-C(29)-C(28)	1.7(2)
C(23)-C(24)-C(29)-C(28)	-175.47(15)
C(25)-C(24)-C(29)-C(20)	-174.40(15)

C(23)-C(24)-C(29)-C(20)	8.5(2)
O(3)-C(20)-C(29)-C(28)	-79.93(19)
C(21)-C(20)-C(29)-C(28)	158.44(15)
O(3)-C(20)-C(29)-C(24)	96.15(19)
C(21)-C(20)-C(29)-C(24)	-25.5(2)
C(30)-C(21)-C(31)-C(32)	46.0(2)
C(20)-C(21)-C(31)-C(32)	-74.32(18)
C(22)-C(21)-C(31)-C(32)	167.35(14)
C(21)-C(31)-C(32)-C(33)	179.32(15)
C(31)-C(32)-C(33)-C(34)	-126.1(2)
C(32)-C(33)-C(34)-C(35)	-1.6(3)
C(32)-C(33)-C(34)-C(36)	177.55(18)
C(23)-C(22)-C(37)-C(38)	105.4(2)
C(21)-C(22)-C(37)-C(38)	-128.3(2)

Symmetry transformations used to generate equivalent atoms:

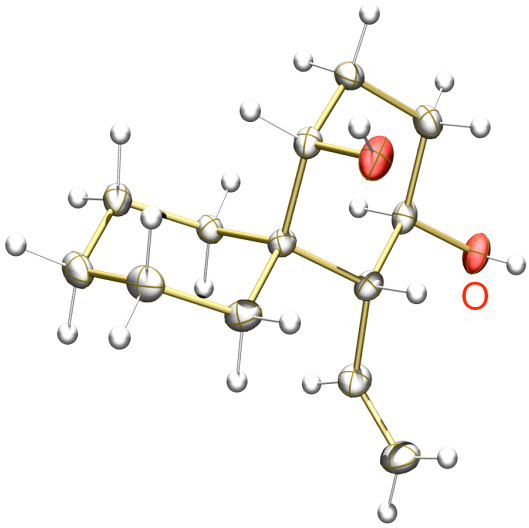
Table 7. Hydrogen bonds for C19H26O2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...O(2)#1	0.851(18)	1.936(18)	2.782(2)	172(2)
O(2)-H(2O)...O(1)#2	0.860(17)	1.931(17)	2.7823(18)	170(3)
O(3)-H(3O)...O(4)#1	0.822(18)	1.860(18)	2.6791(19)	174(2)
O(4)-H(4O)...O(3)#3	0.854(17)	1.832(17)	2.6826(18)	173(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z #2 -x,y-1/2,-z+1 #3 -x+1,y-1/2,-z+2

(1R,4S,5S)-5-vinylspiro[5.5]undecane-1,4-diol (4f)



(*S,S*)-di-*iso*-propylTADDOL-PPh used when this crystal was obtained

Table 1. Crystal data and structure refinement for sad.

Identification code	C13H22O2	
Empirical formula	C13 H22 O2	
Formula weight	210.31	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 7.9329(3) Å	α= 90°.
	b = 7.1935(3) Å	β= 90.3910(10)°.
	c = 10.3786(4) Å	γ = 90°.
Volume	592.24(4) $Å^3$	
Z	2	
Density (calculated)	1.179 Mg/m^3	
Absorption coefficient	0.605 mm^{-1}	
F(000)	232	
Crystal size	0.16 x 0.10 x 0.06 mm^3	
Theta range for data collection	4.26 to 67.51°.	
Index ranges	-9<=h<=8, -8<=k<=8, -12<=l<=12	
Reflections collected	5618	
Independent reflections	2067 [R(int) = 0.0261]	
Completeness to theta = 67.51°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9646 and 0.9094	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2067 / 3 / 142
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0296, wR2 = 0.0792
R indices (all data)	R1 = 0.0299, wR2 = 0.0793
Absolute structure parameter	0.18(18)
Extinction coefficient	na
Largest diff. peak and hole	0.191 and -0.156 e.$Å^{-3}$

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

	x	y	z	U(eq)
O(1)	5229(1)	4949(1)	3638(1)	27(1)
O(2)	4686(1)	11258(1)	3885(1)	26(1)
C(1)	5238(2)	5766(2)	2377(1)	19(1)
C(2)	3574(2)	6790(2)	2153(1)	22(1)
C(3)	3388(2)	8456(2)	3056(1)	24(1)
C(4)	4910(2)	9742(2)	3010(1)	20(1)
C(5)	6561(2)	8676(2)	3273(1)	18(1)
C(6)	6787(2)	7072(2)	2271(1)	17(1)
C(7)	8037(2)	9988(2)	3348(1)	25(1)
C(8)	8921(2)	10330(2)	4401(2)	32(1)
C(9)	6945(2)	7859(2)	889(1)	18(1)
C(10)	7393(2)	6405(2)	-124(1)	22(1)
C(11)	8991(2)	5343(2)	236(1)	27(1)
C(12)	8835(2)	4498(2)	1575(1)	26(1)
C(13)	8412(2)	5980(2)	2583(1)	23(1)

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

O(1)-C(1)	1.4351(15)
O(1)-H(1O)	0.796(16)
O(2)-C(4)	1.4311(15)
O(2)-H(2O)	0.809(14)
C(1)-C(2)	1.5282(17)
C(1)-C(6)	1.5505(15)
C(1)-H(1)	1.0000
C(2)-C(3)	1.5293(18)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.5221(17)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.5414(17)
C(4)-H(4)	1.0000
C(5)-C(7)	1.5056(17)
C(5)-C(6)	1.5646(16)
C(5)-H(5)	1.0000
C(6)-C(13)	1.5426(16)
C(6)-C(9)	1.5482(16)
C(7)-C(8)	1.318(2)
C(7)-H(7A)	0.9500
C(8)-H(8A)	0.9500
C(8)-H(8C)	0.9500
C(9)-C(10)	1.5267(17)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.5245(18)
C(10)-H(10A)	0.9900
C(10)-H(10C)	0.9900
C(11)-C(12)	1.522(2)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.5325(18)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900

C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900

C(1)-O(1)-H(1O)	108.9(14)
C(4)-O(2)-H(2O)	110.0(14)
O(1)-C(1)-C(2)	109.04(10)
O(1)-C(1)-C(6)	108.76(9)
C(2)-C(1)-C(6)	112.41(10)
O(1)-C(1)-H(1)	108.9
C(2)-C(1)-H(1)	108.9
C(6)-C(1)-H(1)	108.9
C(1)-C(2)-C(3)	111.80(10)
C(1)-C(2)-H(2A)	109.3
C(3)-C(2)-H(2A)	109.3
C(1)-C(2)-H(2B)	109.3
C(3)-C(2)-H(2B)	109.3
H(2A)-C(2)-H(2B)	107.9
C(4)-C(3)-C(2)	112.14(10)
C(4)-C(3)-H(3A)	109.2
C(2)-C(3)-H(3A)	109.2
C(4)-C(3)-H(3B)	109.2
C(2)-C(3)-H(3B)	109.2
H(3A)-C(3)-H(3B)	107.9
O(2)-C(4)-C(3)	109.95(10)
O(2)-C(4)-C(5)	112.06(10)
C(3)-C(4)-C(5)	111.42(10)
O(2)-C(4)-H(4)	107.7
C(3)-C(4)-H(4)	107.7
C(5)-C(4)-H(4)	107.7
C(7)-C(5)-C(4)	110.90(10)
C(7)-C(5)-C(6)	113.85(10)
C(4)-C(5)-C(6)	110.48(10)
C(7)-C(5)-H(5)	107.1
C(4)-C(5)-H(5)	107.1
C(6)-C(5)-H(5)	107.1
C(13)-C(6)-C(9)	107.93(9)
C(13)-C(6)-C(1)	109.78(10)
C(9)-C(6)-C(1)	110.88(9)

C(13)-C(6)-C(5)	109.57(9)
C(9)-C(6)-C(5)	110.87(10)
C(1)-C(6)-C(5)	107.79(9)
C(8)-C(7)-C(5)	124.65(13)
C(8)-C(7)-H(7A)	117.7
C(5)-C(7)-H(7A)	117.7
C(7)-C(8)-H(8A)	120.0
C(7)-C(8)-H(8C)	120.0
H(8A)-C(8)-H(8C)	120.0
C(10)-C(9)-C(6)	114.06(10)
C(10)-C(9)-H(9A)	108.7
C(6)-C(9)-H(9A)	108.7
C(10)-C(9)-H(9B)	108.7
C(6)-C(9)-H(9B)	108.7
H(9A)-C(9)-H(9B)	107.6
C(11)-C(10)-C(9)	111.84(10)
C(11)-C(10)-H(10A)	109.2
C(9)-C(10)-H(10A)	109.2
C(11)-C(10)-H(10C)	109.2
C(9)-C(10)-H(10C)	109.2
H(10A)-C(10)-H(10C)	107.9
C(12)-C(11)-C(10)	110.55(10)
C(12)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11A)	109.5
C(12)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	108.1
C(11)-C(12)-C(13)	111.41(11)
C(11)-C(12)-H(12A)	109.3
C(13)-C(12)-H(12A)	109.3
C(11)-C(12)-H(12B)	109.3
C(13)-C(12)-H(12B)	109.3
H(12A)-C(12)-H(12B)	108.0
C(12)-C(13)-C(6)	113.41(10)
C(12)-C(13)-H(13A)	108.9
C(6)-C(13)-H(13A)	108.9
C(12)-C(13)-H(13B)	108.9
C(6)-C(13)-H(13B)	108.9

H(13A)-C(13)-H(13B)	107.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sad. 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)	44(1)	16(1)	21(1)	2(1)	4(1)	-6(1)
O(2)	40(1)	16(1)	21(1)	-2(1)	3(1)	4(1)
C(1)	23(1)	15(1)	18(1)	0(1)	2(1)	-3(1)
C(2)	18(1)	22(1)	25(1)	-3(1)	2(1)	-4(1)
C(3)	21(1)	23(1)	26(1)	-1(1)	4(1)	2(1)
C(4)	27(1)	14(1)	18(1)	-2(1)	2(1)	2(1)
C(5)	24(1)	14(1)	18(1)	0(1)	-1(1)	-2(1)
C(6)	18(1)	13(1)	18(1)	-1(1)	-1(1)	0(1)
C(7)	28(1)	18(1)	28(1)	-1(1)	1(1)	-5(1)
C(8)	30(1)	28(1)	38(1)	-7(1)	-6(1)	-5(1)
C(9)	17(1)	16(1)	20(1)	0(1)	2(1)	0(1)
C(10)	24(1)	20(1)	22(1)	-1(1)	4(1)	-3(1)
C(11)	22(1)	21(1)	38(1)	-7(1)	7(1)	0(1)
C(12)	22(1)	17(1)	38(1)	-4(1)	-2(1)	4(1)
C(13)	22(1)	19(1)	28(1)	-1(1)	-6(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for sad.

	x	y	z	U(eq)
H(1O)	5120(20)	3850(20)	3568(19)	40
H(2O)	4670(20)	10880(30)	4619(14)	39
H(1)	5343	4754	1722	22
H(2A)	2626	5920	2291	26
H(2B)	3518	7225	1249	26
H(3A)	2364	9164	2812	28
H(3B)	3241	8003	3949	28
H(4)	4973	10269	2120	23
H(5)	6452	8082	4140	22
H(7A)	8354	10615	2581	30
H(8A)	8641	9729	5186	38
H(8C)	9839	11178	4376	38
H(9A)	5863	8450	642	21
H(9B)	7822	8839	890	21
H(10A)	6447	5517	-217	26
H(10C)	7555	7026	-965	26
H(11A)	9188	4344	-401	32
H(11B)	9969	6197	217	32
H(12A)	9910	3884	1814	31
H(12B)	7940	3539	1565	31
H(13A)	9365	6865	2649	28
H(13B)	8288	5371	3433	28

Table 6. Torsion angles [°] for sad.

O(1)-C(1)-C(2)-C(3)	65.73(13)
C(6)-C(1)-C(2)-C(3)	-54.96(13)
C(1)-C(2)-C(3)-C(4)	52.25(14)
C(2)-C(3)-C(4)-O(2)	-179.07(10)
C(2)-C(3)-C(4)-C(5)	-54.21(14)
O(2)-C(4)-C(5)-C(7)	-51.03(14)
C(3)-C(4)-C(5)-C(7)	-174.69(10)
O(2)-C(4)-C(5)-C(6)	-178.23(10)
C(3)-C(4)-C(5)-C(6)	58.10(13)
O(1)-C(1)-C(6)-C(13)	55.92(12)
C(2)-C(1)-C(6)-C(13)	176.77(10)
O(1)-C(1)-C(6)-C(9)	175.09(10)
C(2)-C(1)-C(6)-C(9)	-64.06(13)
O(1)-C(1)-C(6)-C(5)	-63.38(12)
C(2)-C(1)-C(6)-C(5)	57.47(12)
C(7)-C(5)-C(6)-C(13)	56.50(13)
C(4)-C(5)-C(6)-C(13)	-177.95(10)
C(7)-C(5)-C(6)-C(9)	-62.54(13)
C(4)-C(5)-C(6)-C(9)	63.02(12)
C(7)-C(5)-C(6)-C(1)	175.92(10)
C(4)-C(5)-C(6)-C(1)	-58.52(12)
C(4)-C(5)-C(7)-C(8)	112.86(15)
C(6)-C(5)-C(7)-C(8)	-121.81(15)
C(13)-C(6)-C(9)-C(10)	52.55(13)
C(1)-C(6)-C(9)-C(10)	-67.72(12)
C(5)-C(6)-C(9)-C(10)	172.57(10)
C(6)-C(9)-C(10)-C(11)	-54.72(14)
C(9)-C(10)-C(11)-C(12)	54.39(14)
C(10)-C(11)-C(12)-C(13)	-55.40(14)
C(11)-C(12)-C(13)-C(6)	56.87(14)
C(9)-C(6)-C(13)-C(12)	-53.46(13)
C(1)-C(6)-C(13)-C(12)	67.51(13)
C(5)-C(6)-C(13)-C(12)	-174.29(10)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for sad [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...O(2)#1	0.796(16)	1.928(16)	2.7024(14)	164(2)
O(2)-H(2O)...O(1)#2	0.809(14)	1.930(15)	2.7381(14)	176.9(19)

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z #2 -x+1,y+1/2,-z+1