Supporting information

An enantioselective synthesis of C(33)-C(37) fragment of Amphotericin B

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Table S1. Crystal data and structure refinement for **7b**.

Identification code	7b	
Empirical formula	C16 H24 O7 S	
Formula weight	360.41	
Temperature	173.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 5.2341(2) Å	α= 90°.
	b = 12.3751(5) Å	β= 97.6880(10)°.
	c = 14.2381(7) Å	γ = 90°.
Volume	913.95(7) $Å^3$	
Z	2	
Density (calculated)	1.310 Mg/m^3	
Absorption coefficient	0.210 mm^{-1}	
F(000)	384	
Crystal size	0.1 x 0.15 x 0.35 mm^3	
Theta range for data collection	2.89 to 25.04°.	
Index ranges	-5<=h<=6, -14<=k<=13, -15<=l<=16	
Reflections collected	5702	
Independent reflections	3175 [R(int) = 0.0303]	
Completeness to theta = 25.04°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3175 / 1 / 222	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0435, wR2 = 0.1030	
R indices (all data)	R1 = 0.0583, wR2 = 0.1099	
Absolute structure parameter	-0.02(11)	
Extinction coefficient	0.022(4)	
Largest diff. peak and hole	0.533 and -0.348 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	6540(2)	-1616(1)	8052(1)	59(1)
O(14)	-1440(4)	3948(2)	7239(2)	33(1)
O(8)	1122(4)	1345(2)	7909(2)	30(1)
O(13)	-780(4)	3186(2)	8691(2)	36(1)
O(11)	4865(3)	1884(2)	7464(2)	33(1)
O(20)	1871(4)	3407(2)	5536(1)	34(1)
O(19)	3884(5)	1799(2)	5533(2)	52(1)
O(4)	3131(6)	541(2)	9959(2)	66(1)
C(9)	444(5)	2249(2)	7324(2)	26(1)
C(12)	-682(5)	3159(2)	7855(2)	26(1)
C(18)	3024(5)	2535(2)	5944(2)	27(1)
C(10)	3050(5)	2614(2)	7002(2)	25(1)
C(7)	3777(5)	1475(3)	8254(2)	31(1)
C(21)	1355(5)	3441(3)	4502(2)	34(1)
C(3)	5109(6)	424(3)	8556(2)	35(1)
C(15)	-2257(6)	4984(3)	7605(2)	33(1)
C(4)	4412(7)	23(3)	9487(2)	42(1)
C(16)	70(7)	5611(3)	8039(3)	47(1)
C(6)	5227(10)	-1952(3)	9125(3)	65(1)
C(23)	1195(8)	4636(3)	4260(3)	52(1)
C(22)	-1071(7)	2838(3)	4181(3)	53(1)
C(2)	4587(8)	-428(3)	7782(3)	50(1)
C(5)	5545(10)	-1055(3)	9835(3)	60(1)
C(17)	-3736(7)	5537(3)	6760(3)	45(1)

Table S3. Bond lengths [Å] and angles [°] for **7b**.

S(1)-C(2)	1.802(4)
S(1)-C(6)	1.805(5)
O(14)-C(12)	1.337(4)
O(14)-C(15)	1.469(4)
O(8)-C(9)	1.411(3)
O(8)-C(7)	1.419(4)
O(13)-C(12)	1.198(4)
O(11)-C(10)	1.408(3)
O(11)-C(7)	1.420(4)
O(20)-C(18)	1.331(4)
O(20)-C(21)	1.460(4)
O(19)-C(18)	1.202(4)
O(4)-C(4)	1.197(4)
C(9)-C(12)	1.519(4)
C(9)-C(10)	1.562(4)
C(18)-C(10)	1.509(4)
C(7)-C(3)	1.511(4)
C(21)-C(22)	1.491(5)
C(21)-C(23)	1.519(5)
C(3)-C(4)	1.505(5)
C(3)-C(2)	1.523(5)
C(15)-C(17)	1.504(5)
C(15)-C(16)	1.505(5)
C(4)-C(5)	1.517(5)
C(6)-C(5)	1.495(6)

C(2)-S(1)-C(6)	95.7(2)
C(12)-O(14)-C(15)	118.7(2)
C(9)-O(8)-C(7)	105.8(2)
C(10)-O(11)-C(7)	106.3(2)
C(18)-O(20)-C(21)	118.3(2)
O(8)-C(9)-C(12)	112.2(2)
O(8)-C(9)-C(10)	104.0(2)
C(12)-C(9)-C(10)	110.1(2)
O(13)-C(12)-O(14)	125.7(3)
O(13)-C(12)-C(9)	125.9(3)

O(14)-C(12)-C(9)	108.4(2)
O(19)-C(18)-O(20)	125.4(3)
O(19)-C(18)-C(10)	125.5(3)
O(20)-C(18)-C(10)	109.1(2)
O(11)-C(10)-C(18)	109.9(2)
O(11)-C(10)-C(9)	103.8(2)
C(18)-C(10)-C(9)	112.5(2)
O(8)-C(7)-O(11)	104.1(2)
O(8)-C(7)-C(3)	113.2(3)
O(11)-C(7)-C(3)	108.3(2)
O(20)-C(21)-C(22)	109.3(3)
O(20)-C(21)-C(23)	104.7(3)
C(22)-C(21)-C(23)	113.5(3)
C(4)-C(3)-C(7)	112.2(3)
C(4)-C(3)-C(2)	111.6(3)
C(7)-C(3)-C(2)	111.0(3)
O(14)-C(15)-C(17)	104.9(3)
O(14)-C(15)-C(16)	109.7(2)
C(17)-C(15)-C(16)	113.3(3)
O(4)-C(4)-C(3)	122.6(3)
O(4)-C(4)-C(5)	120.8(3)
C(3)-C(4)-C(5)	116.5(3)
C(5)-C(6)-S(1)	112.4(3)
C(3)-C(2)-S(1)	111.6(2)
C(6)-C(5)-C(4)	115.4(3)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **7b**. 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}
S(1)	90(1)	41(1)	46(1)	0(1)	11(1)	32(1)
O(14)	40(1)	24(1)	36(1)	3(1)	11(1)	8(1)
O(8)	32(1)	19(1)	42(1)	4(1)	10(1)	3(1)
O(13)	45(1)	35(1)	29(1)	0(1)	5(1)	7(1)
O(11)	23(1)	39(1)	36(1)	14(1)	5(1)	8(1)
O(20)	38(1)	35(1)	29(1)	7(1)	4(1)	9(1)
O(19)	70(2)	48(2)	39(2)	4(1)	14(1)	29(1)
O(4)	113(2)	46(2)	45(2)	7(1)	36(2)	27(2)
C(9)	24(1)	23(2)	32(2)	1(1)	6(1)	1(1)
C(12)	24(1)	22(2)	34(2)	1(1)	4(1)	-1(1)
C(18)	23(1)	29(2)	30(2)	3(1)	4(1)	-1(1)
C(10)	22(1)	21(2)	32(2)	3(1)	2(1)	0(1)
C(7)	30(2)	34(2)	30(2)	5(1)	4(1)	7(1)
C(21)	30(2)	42(2)	29(2)	5(2)	2(1)	2(2)
C(3)	44(2)	29(2)	33(2)	4(2)	5(1)	9(1)
C(15)	35(2)	24(2)	44(2)	-1(1)	14(1)	6(1)
C(4)	57(2)	38(2)	29(2)	1(2)	6(2)	11(2)
C(16)	45(2)	30(2)	65(3)	-6(2)	2(2)	3(2)
C(6)	97(3)	28(2)	73(3)	15(2)	23(3)	11(2)
C(23)	60(2)	48(2)	47(2)	15(2)	-2(2)	-7(2)
C(22)	47(2)	53(2)	55(2)	13(2)	-9(2)	-10(2)
C(2)	67(2)	44(2)	37(2)	-3(2)	-3(2)	14(2)
C(5)	95(3)	44(2)	45(2)	11(2)	21(2)	19(2)
C(17)	48(2)	29(2)	60(2)	9(2)	9(2)	5(2)

Table S5. Torsion angles [°] for **7b**.

C(7)-O(8)-C(9)-C(12)	-94.4(3)
C(7)-O(8)-C(9)-C(10)	24.5(3)
C(15)-O(14)-C(12)-O(13)	5.8(4)
C(15)-O(14)-C(12)-C(9)	-171.4(2)
O(8)-C(9)-C(12)-O(13)	7.2(4)
C(10)-C(9)-C(12)-O(13)	-108.1(3)
O(8)-C(9)-C(12)-O(14)	-175.6(2)
C(10)-C(9)-C(12)-O(14)	69.1(3)
C(21)-O(20)-C(18)-O(19)	6.6(4)
C(21)-O(20)-C(18)-C(10)	-172.8(2)
C(7)-O(11)-C(10)-C(18)	-143.1(2)
C(7)-O(11)-C(10)-C(9)	-22.6(3)
O(19)-C(18)-C(10)-O(11)	17.5(4)
O(20)-C(18)-C(10)-O(11)	-163.1(2)
O(19)-C(18)-C(10)-C(9)	-97.6(3)
O(20)-C(18)-C(10)-C(9)	81.8(3)
O(8)-C(9)-C(10)-O(11)	-1.2(3)
C(12)-C(9)-C(10)-O(11)	119.1(3)
O(8)-C(9)-C(10)-C(18)	117.5(2)
C(12)-C(9)-C(10)-C(18)	-122.2(3)
C(9)-O(8)-C(7)-O(11)	-39.5(3)
C(9)-O(8)-C(7)-C(3)	-156.9(2)
C(10)-O(11)-C(7)-O(8)	38.8(3)
C(10)-O(11)-C(7)-C(3)	159.6(2)
C(18)-O(20)-C(21)-C(22)	82.3(3)
C(18)-O(20)-C(21)-C(23)	-155.8(3)
O(8)-C(7)-C(3)-C(4)	-74.8(4)
O(11)-C(7)-C(3)-C(4)	170.3(3)
O(8)-C(7)-C(3)-C(2)	50.8(4)
O(11)-C(7)-C(3)-C(2)	-64.1(3)
C(12)-O(14)-C(15)-C(17)	-162.6(2)
C(12)-O(14)-C(15)-C(16)	75.4(3)
C(7)-C(3)-C(4)-O(4)	-6.2(5)
C(2)-C(3)-C(4)-O(4)	-131.5(4)
C(7)-C(3)-C(4)-C(5)	177.2(3)
C(2)-C(3)-C(4)-C(5)	51.9(4)

C(2)-S(1)-C(6)-C(5)	-57.8(4)
C(4)-C(3)-C(2)-S(1)	-62.9(4)
C(7)-C(3)-C(2)-S(1)	171.2(2)
C(6)-S(1)-C(2)-C(3)	61.8(3)
S(1)-C(6)-C(5)-C(4)	56.1(5)
O(4)-C(4)-C(5)-C(6)	133.8(4)
C(3)-C(4)-C(5)-C(6)	-49.5(5)

Symmetry transformations used to generate equivalent atoms: