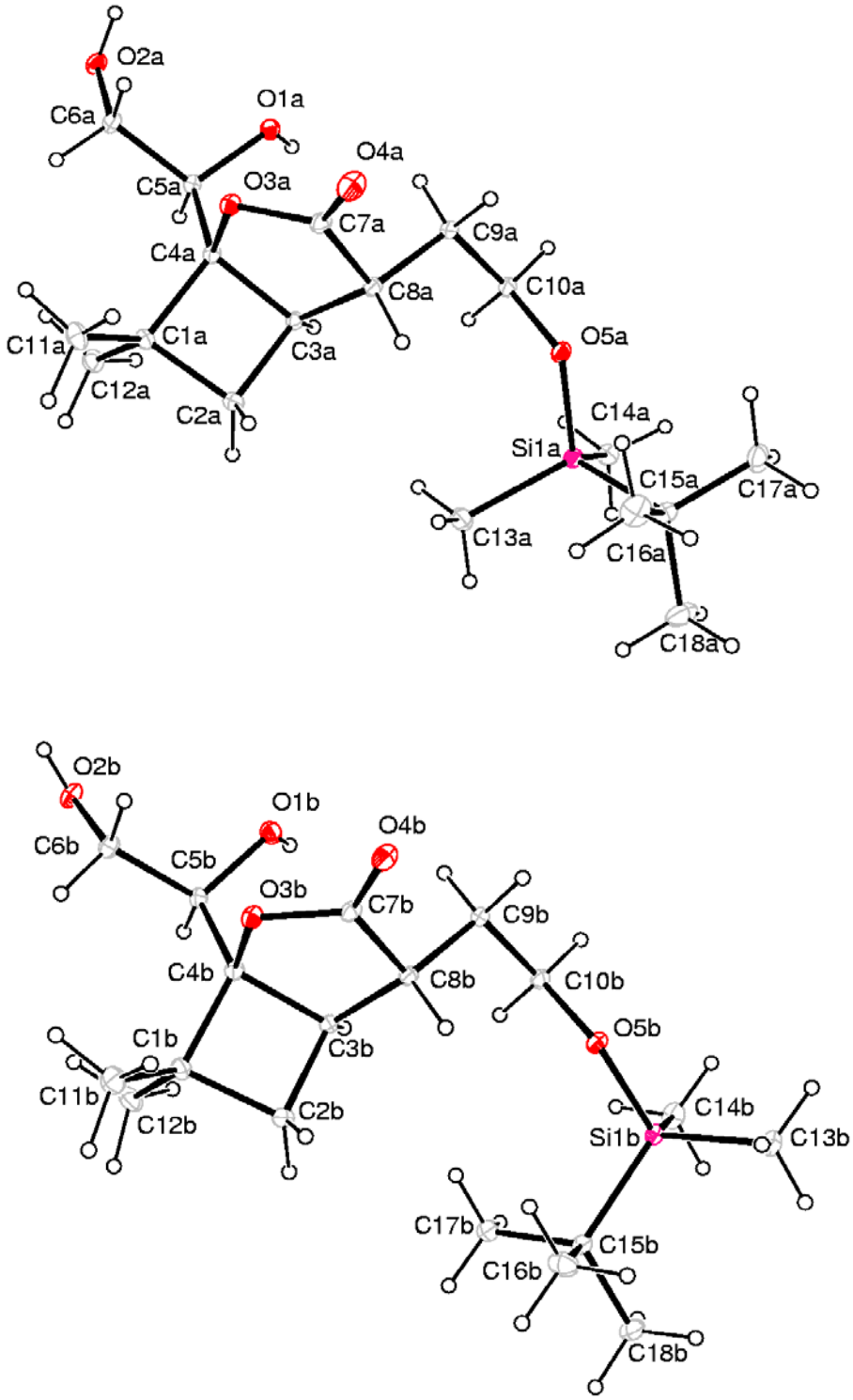
Supplementary Material for "The first synthetic studies on pestalotiopsin A. A stereocontrolled approach to the functionalised bicyclic core."
Crystal Structure Analysis of 18a $C_{18}H_{34}O_5Si$

Fig. S1. 18a –(20% ellipsoids). The crystal contains two independent molecules which differ mainly in the conformation across the O5-Si bonds.



- **Table S1. Crystal data and structure refinement for 18a.**
- **Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 18a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.**
- **Table S3. Bond lengths [Å] and angles [°] for 18a.**
- **Table S4. Anisotropic displacement parameters (Å^{2}x 10^3)for 18a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$**
- **Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3)for 18a.**
- **Table S6. Torsion angles [°] for 18a.**
- **Table S7. Hydrogen bonds for 18a [Å and °].**

Table S1. Crystal data and structure refinement for 18a.

Identification code	18a	
Empirical formula	$C_{18} H_{34} O_5 Si$	
Formula weight	358.54	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.6770(2) Å	α= 102.147(1)°.
	b = 12.7397(2) Å	β= 95.218(1)°.
	c = 13.0974(2) Å	γ = 91.166(1)°.
Volume	2057.62(6) $Å^3$	
Z	4	
Density (calculated)	1.157 Mg/m^3	
Absorption coefficient	0.136 mm^{-1}	
F(000)	784	
Crystal size	0.55 x 0.20 x 0.10 mm^3	
Theta range for data collection	2.03 to 27.50°.	
Index ranges	-16<=h<=16, -16<=k<=16, 0<=l<=16	
Reflections collected	31303	
Independent reflections	9393 [R(int) = 0.0275]	
Completeness to theta = 27.50°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.996 and 0.909	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9393 / 0 / 445	
Goodness-of-fit on F^2	1.040	
R indices [7639 I>2σ(I)]	R1 = 0.0374, wR2 = 0.0871	
R indices (all data)	R1 = 0.0492, wR2 = 0.0939	
Largest diff. peak and hole	0.53 and -0.24 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 18a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1A)	2421(1)	14272(1)	5510(1)	19(1)
O(1A)	461(1)	11301(1)	910(1)	21(1)
O(2A)	398(1)	10574(1)	-1295(1)	24(1)
O(3A)	2472(1)	10511(1)	1391(1)	19(1)
O(4A)	2585(1)	9837(1)	2830(1)	35(1)
O(5A)	1794(1)	13098(1)	5037(1)	21(1)
C(1A)	3437(1)	11951(1)	788(1)	20(1)
C(2A)	3652(1)	12594(1)	1941(1)	22(1)
C(3A)	2485(1)	12382(1)	2142(1)	16(1)
C(4A)	2357(1)	11542(1)	1088(1)	17(1)
C(5A)	1352(1)	11476(1)	359(1)	18(1)
C(6A)	1343(1)	10577(1)	-610(1)	22(1)
C(7A)	2482(1)	10608(1)	2444(1)	21(1)
C(8A)	2331(1)	11758(1)	2995(1)	19(1)
C(9A)	1245(1)	11822(1)	3435(1)	22(1)
C(10A)	1066(1)	12911(1)	4108(1)	21(1)
C(11A)	4221(1)	11097(1)	422(1)	29(1)
C(12A)	3290(1)	12703(1)	22(1)	26(1)

C(13A)	3394(1)	14522(1)	4584(1)	29(1)
C(14A)	1458(1)	15360(1)	5653(1)	25(1)
C(15A)	3110(1)	14131(1)	6809(1)	25(1)
C(16A)	3846(1)	13183(1)	6650(1)	39(1)
C(17A)	2281(1)	13920(1)	7537(1)	34(1)
C(18A)	3758(2)	15167(1)	7328(1)	43(1)
Si(1B)	2186(1)	8898(1)	6302(1)	18(1)
O(1B)	143(1)	7260(1)	1058(1)	25(1)
O(2B)	367(1)	6742(1)	-1193(1)	24(1)
O(3B)	1504(1)	5649(1)	1497(1)	20(1)
O(4B)	711(1)	4939(1)	2656(1)	27(1)
O(5B)	1471(1)	8063(1)	5335(1)	21(1)
C(1B)	3127(1)	6695(1)	1269(1)	22(1)
C(2B)	3315(1)	7081(1)	2484(1)	24(1)
C(3B)	2128(1)	7343(1)	2528(1)	18(1)
C(4B)	1910(1)	6701(1)	1384(1)	18(1)
C(5B)	1122(1)	7090(1)	610(1)	18(1)
C(6B)	957(1)	6277(1)	-430(1)	22(1)
C(7B)	1180(1)	5701(1)	2459(1)	19(1)
C(8B)	1497(1)	6767(1)	3196(1)	18(1)
C(9B)	533(1)	7345(1)	3638(1)	21(1)
C(10B)	851(1)	8349(1)	4475(1)	21(1)
C(11B)	3586(1)	5629(1)	804(1)	32(1)
C(12B)	3480(1)	7578(1)	729(1)	31(1)
C(13B)	2055(1)	8352(1)	7500(1)	25(1)
C(14B)	1680(1)	10282(1)	6457(1)	29(1)
C(15B)	3614(1)	8884(1)	5997(1)	23(1)
C(16B)	4009(1)	7740(1)	5877(1)	35(1)
C(17B)	3693(1)	9244(1)	4959(1)	32(1)
C(18B)	4322(1)	9641(1)	6875(1)	32(1)

Table S3. Bond lengths [Å] and angles [°] for 18a

Si(1A)-O(5A)	1.6511(10)	C(15A)-C(17A)	1.537(2)
Si(1A)-C(14A)	1.8563(14)	Si(1B)-O(5B)	1.6565(10)
Si(1A)-C(13A)	1.8732(15)	Si(1B)-C(13B)	1.8642(14)
Si(1A)-C(15A)	1.8851(14)	Si(1B)-C(14B)	1.8647(15)
O(1A)-C(5A)	1.4322(15)	Si(1B)-C(15B)	1.8886(14)
O(2A)-C(6A)	1.4294(16)	O(1B)-C(5B)	1.4219(16)
O(3A)-C(7A)	1.3573(16)	O(2B)-C(6B)	1.4284(16)
O(3A)-C(4A)	1.4560(15)	O(3B)-C(7B)	1.3487(15)
O(4A)-C(7A)	1.2000(16)	O(3B)-C(4B)	1.4662(15)
O(5A)-C(10A)	1.4333(15)	O(4B)-C(7B)	1.2130(16)
C(1A)-C(11A)	1.5207(19)	O(5B)-C(10B)	1.4288(15)
C(1A)-C(12A)	1.5294(18)	C(1B)-C(11B)	1.517(2)
C(1A)-C(2A)	1.5562(18)	C(1B)-C(12B)	1.529(2)
C(1A)-C(4A)	1.5667(17)	C(1B)-C(2B)	1.5586(19)
C(2A)-C(3A)	1.5543(18)	C(1B)-C(4B)	1.5645(18)
C(3A)-C(8A)	1.5250(17)	C(2B)-C(3B)	1.5520(18)
C(3A)-C(4A)	1.5518(17)	C(3B)-C(8B)	1.5224(17)
C(4A)-C(5A)	1.5118(18)	C(3B)-C(4B)	1.5454(17)
C(5A)-C(6A)	1.5185(17)	C(4B)-C(5B)	1.5231(18)
C(7A)-C(8A)	1.5144(18)	C(5B)-C(6B)	1.5223(18)
C(8A)-C(9A)	1.5374(19)	C(7B)-C(8B)	1.5146(18)
C(9A)-C(10A)	1.5127(19)	C(8B)-C(9B)	1.5347(19)
C(15A)-C(16A)	1.533(2)	C(9B)-C(10B)	1.5188(18)
C(15A)-C(18A)	1.535(2)	C(15B)-C(16B)	1.532(2)

C(15B)-C(17B)	1.5342(19)	C(15B)-C(18B)	1.5390(19)

O(5A)-Si(1A)-C(14A)	110.01(6)	O(5B)-Si(1B)-C(13B)	105.75(6)
O(5A)-Si(1A)-C(13A)	109.27(6)	O(5B)-Si(1B)-C(14B)	110.35(6)
C(14A)-Si(1A)-C(13A)	109.02(7)	C(13B)-Si(1B)-C(14B)	111.32(7)
O(5A)-Si(1A)-C(15A)	104.36(6)	O(5B)-Si(1B)-C(15B)	108.50(6)
C(14A)-Si(1A)-C(15A)	112.48(6)	C(13B)-Si(1B)-C(15B)	110.05(7)
C(13A)-Si(1A)-C(15A)	111.59(7)	C(14B)-Si(1B)-C(15B)	110.73(7)
C(7A)-O(3A)-C(4A)	111.89(10)	C(7B)-O(3B)-C(4B)	111.25(10)
C(10A)-O(5A)-Si(1A)	122.11(8)	C(10B)-O(5B)-Si(1B)	126.38(8)
C(11A)-C(1A)-C(12A)	110.63(11)	C(11B)-C(1B)-C(12B)	111.07(12)
C(11A)-C(1A)-C(2A)	116.35(12)	C(11B)-C(1B)-C(2B)	116.40(12)
C(12A)-C(1A)-C(2A)	111.31(11)	C(12B)-C(1B)-C(2B)	110.35(12)
C(11A)-C(1A)-C(4A)	116.44(11)	C(11B)-C(1B)-C(4B)	117.40(12)
C(12A)-C(1A)-C(4A)	112.63(11)	C(12B)-C(1B)-C(4B)	111.93(11)
C(2A)-C(1A)-C(4A)	87.79(9)	C(2B)-C(1B)-C(4B)	87.76(9)
C(3A)-C(2A)-C(1A)	90.83(9)	C(3B)-C(2B)-C(1B)	90.24(10)
C(8A)-C(3A)-C(4A)	106.02(10)	C(8B)-C(3B)-C(4B)	106.69(10)
C(8A)-C(3A)-C(2A)	115.91(11)	C(8B)-C(3B)-C(2B)	116.76(11)
C(4A)-C(3A)-C(2A)	88.39(9)	C(4B)-C(3B)-C(2B)	88.68(10)
O(3A)-C(4A)-C(5A)	108.19(10)	O(3B)-C(4B)-C(5B)	107.09(10)
O(3A)-C(4A)-C(3A)	104.51(9)	O(3B)-C(4B)-C(3B)	103.71(10)
C(5A)-C(4A)-C(3A)	120.04(11)	C(5B)-C(4B)-C(3B)	120.52(11)
O(3A)-C(4A)-C(1A)	110.57(10)	O(3B)-C(4B)-C(1B)	111.35(10)
C(5A)-C(4A)-C(1A)	121.17(10)	C(5B)-C(4B)-C(1B)	122.07(11)
C(3A)-C(4A)-C(1A)	90.53(9)	C(3B)-C(4B)-C(1B)	90.26(10)
O(1A)-C(5A)-C(4A)	109.22(10)	O(1B)-C(5B)-C(6B)	110.07(11)
O(1A)-C(5A)-C(6A)	108.48(10)	O(1B)-C(5B)-C(4B)	108.67(10)
C(4A)-C(5A)-C(6A)	112.86(11)	C(6B)-C(5B)-C(4B)	111.13(11)
O(2A)-C(6A)-C(5A)	110.81(11)	O(2B)-C(6B)-C(5B)	109.64(11)
O(4A)-C(7A)-O(3A)	120.70(12)	O(4B)-C(7B)-O(3B)	120.49(12)
O(4A)-C(7A)-C(8A)	127.73(12)	O(4B)-C(7B)-C(8B)	127.40(12)
O(3A)-C(7A)-C(8A)	111.56(11)	O(3B)-C(7B)-C(8B)	112.10(10)
C(7A)-C(8A)-C(3A)	102.73(10)	C(7B)-C(8B)-C(3B)	102.68(10)
C(7A)-C(8A)-C(9A)	108.83(11)	C(7B)-C(8B)-C(9B)	111.94(11)
C(3A)-C(8A)-C(9A)	116.67(11)	C(3B)-C(8B)-C(9B)	116.13(11)
C(10A)-C(9A)-C(8A)	113.13(11)	C(10B)-C(9B)-C(8B)	112.34(11)
O(5A)-C(10A)-C(9A)	109.37(11)	O(5B)-C(10B)-C(9B)	109.63(11)
C(16A)-C(15A)-C(18A)	109.53(13)	C(16B)-C(15B)-C(17B)	108.50(13)
C(16A)-C(15A)-C(17A)	108.40(13)	C(16B)-C(15B)-C(18B)	109.18(12)
C(18A)-C(15A)-C(17A)	109.07(13)	C(17B)-C(15B)-C(18B)	109.15(12)
C(16A)-C(15A)-Si(1A)	110.23(10)	C(16B)-C(15B)-Si(1B)	109.63(10)
C(18A)-C(15A)-Si(1A)	109.97(10)	C(17B)-C(15B)-Si(1B)	109.36(10)
C(17A)-C(15A)-Si(1A)	109.61(10)	C(18B)-C(15B)-Si(1B)	110.97(10)

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3)for 18a. 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}
Si(1A)	19(1)	19(1)	18(1)	3(1)	2(1)	1(1)
O(1A)	20(1)	21(1)	22(1)	2(1)	4(1)	2(1)
O(2A)	26(1)	26(1)	18(1)	2(1)	-2(1)	-1(1)
O(3A)	25(1)	14(1)	18(1)	3(1)	2(1)	3(1)
O(4A)	60(1)	19(1)	28(1)	10(1)	-1(1)	2(1)

O(5A)	25(1)	22(1)	16(1)	3(1)	-1(1)	-1(1)
C(1A)	19(1)	21(1)	21(1)	5(1)	5(1)	2(1)
C(2A)	20(1)	25(1)	23(1)	5(1)	2(1)	-3(1)
C(3A)	18(1)	15(1)	16(1)	3(1)	1(1)	0(1)
C(4A)	21(1)	13(1)	16(1)	4(1)	3(1)	3(1)
C(5A)	20(1)	19(1)	17(1)	3(1)	3(1)	2(1)
C(6A)	23(1)	23(1)	18(1)	0(1)	1(1)	3(1)
C(7A)	26(1)	18(1)	20(1)	4(1)	0(1)	-1(1)
C(8A)	23(1)	17(1)	16(1)	3(1)	0(1)	-1(1)
C(9A)	26(1)	24(1)	16(1)	3(1)	2(1)	-7(1)
C(10A)	20(1)	27(1)	16(1)	4(1)	1(1)	-1(1)
C(11A)	25(1)	33(1)	32(1)	8(1)	12(1)	8(1)
C(12A)	31(1)	24(1)	25(1)	8(1)	6(1)	0(1)
C(13A)	29(1)	27(1)	30(1)	4(1)	8(1)	-1(1)
C(14A)	26(1)	22(1)	26(1)	5(1)	2(1)	2(1)
C(15A)	24(1)	25(1)	23(1)	3(1)	-4(1)	0(1)
C(16A)	33(1)	44(1)	40(1)	11(1)	-4(1)	14(1)
C(17A)	38(1)	45(1)	21(1)	11(1)	1(1)	4(1)
C(18A)	48(1)	40(1)	37(1)	9(1)	-18(1)	-12(1)
Si(1B)	22(1)	18(1)	15(1)	2(1)	1(1)	0(1)
O(1B)	23(1)	29(1)	23(1)	7(1)	4(1)	4(1)
O(2B)	33(1)	21(1)	16(1)	3(1)	-4(1)	1(1)
O(3B)	27(1)	15(1)	17(1)	3(1)	1(1)	-2(1)
O(4B)	36(1)	23(1)	21(1)	8(1)	-2(1)	-8(1)
O(5B)	23(1)	22(1)	17(1)	4(1)	-2(1)	-1(1)
C(1B)	21(1)	23(1)	22(1)	2(1)	5(1)	2(1)
C(2B)	18(1)	30(1)	24(1)	1(1)	1(1)	0(1)
C(3B)	18(1)	18(1)	17(1)	1(1)	1(1)	-2(1)
C(4B)	21(1)	14(1)	18(1)	2(1)	3(1)	-2(1)
C(5B)	22(1)	18(1)	16(1)	4(1)	3(1)	1(1)
C(6B)	28(1)	20(1)	18(1)	4(1)	0(1)	3(1)
C(7B)	22(1)	20(1)	16(1)	5(1)	-2(1)	0(1)
C(8B)	20(1)	20(1)	15(1)	3(1)	-1(1)	-2(1)
C(9B)	18(1)	29(1)	16(1)	4(1)	1(1)	-2(1)
C(10B)	19(1)	27(1)	17(1)	5(1)	1(1)	4(1)
C(11B)	30(1)	31(1)	32(1)	0(1)	5(1)	11(1)
C(12B)	26(1)	33(1)	34(1)	7(1)	11(1)	-2(1)
C(13B)	34(1)	25(1)	17(1)	4(1)	4(1)	0(1)
C(14B)	37(1)	24(1)	27(1)	4(1)	3(1)	6(1)
C(15B)	21(1)	26(1)	19(1)	4(1)	-1(1)	-3(1)
C(16B)	25(1)	34(1)	44(1)	5(1)	4(1)	6(1)
C(17B)	26(1)	47(1)	24(1)	10(1)	1(1)	-9(1)
C(18B)	28(1)	40(1)	26(1)	5(1)	-5(1)	-8(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 18a.

	x	y	z	U(eq)
H(1A)	151(14)	11885(15)	1034(13)	32
H(2A)	14(15)	10057(15)	-1219(14)	36
H(2A1)	4176	12265	2373	27
H(2A2)	3841	13364	1999	27
H(3A)	2026	13014	2160	20
H(5A)	1276	12174	131	22

H(6A1)	1969	10671	-986	26
H(6A2)	1387	9877	-395	26
H(8A)	2903	11983	3585	23
H(9A1)	682	11657	2843	26
H(9A2)	1186	11269	3859	26
H(10A)	1173	13478	3710	25
H(10B)	328	12936	4302	25
H(11A)	4920	11442	423	44
H(11B)	3979	10704	-290	44
H(11C)	4271	10597	897	44
H(12A)	3043	12283	-679	39
H(12B)	3967	13076	-5	39
H(12C)	2765	13232	257	39
H(13A)	3014	14543	3904	43
H(13B)	3896	13943	4494	43
H(13C)	3780	15210	4871	43
H(14A)	967	15253	6162	37
H(14B)	1060	15344	4973	37
H(14C)	1840	16056	5901	37
H(16A)	4161	13087	7334	58
H(16B)	4409	13328	6228	58
H(16C)	3437	12528	6288	58
H(17A)	1773	14495	7607	51
H(17B)	2636	13902	8229	51
H(17C)	1904	13229	7238	51
H(18A)	4290	15305	6869	65
H(18B)	4112	15088	8003	65
H(18C)	3284	15771	7443	65
H(1B)	52(14)	8009(16)	1205(14)	37
H(2B)	30(15)	6271(15)	-1601(15)	36
H(2B1)	3531	6504	2852	29
H(2B2)	3803	7720	2714	29
H(3B)	1990	8125	2618	22
H(5B)	1400	7786	482	22
H(6B1)	1652	6060	-674	26
H(6B2)	568	5627	-336	26
H(8B)	1985	6631	3795	22
H(9B1)	80	7546	3058	25
H(9B2)	110	6847	3942	25
H(10C)	1266	8856	4175	25
H(10D)	208	8708	4723	25
H(11D)	4360	5715	845	48
H(11E)	3301	5393	68	48
H(11F)	3394	5091	1197	48
H(12D)	3258	7370	-25	46
H(12E)	4253	7679	839	46
H(12F)	3154	8251	1026	46
H(13D)	2228	7592	7360	38
H(13E)	1325	8422	7689	38
H(13F)	2542	8755	8080	38
H(14D)	950	10278	6644	44
H(14E)	1699	10522	5795	44
H(14F)	2127	10772	7012	44
H(16D)	3978	7504	6539	52
H(16E)	4743	7730	5696	52
H(16F)	3560	7255	5319	52

H(17D)	4426	9197	4778	48
H(17E)	3476	9989	5035	48
H(17F)	3227	8778	4401	48
H(18D)	5064	9583	6723	48
H(18E)	4242	9440	7546	48
H(18F)	4110	10383	6914	48

Table S6. Torsion angles [°] for 18a.

C(14A)-Si(1A)-O(5A)-C(10A)	51.50(11)	C(14A)-Si(1A)-C(15A)-C(18A)	-62.39(13)
C(13A)-Si(1A)-O(5A)-C(10A)	-68.15(11)	C(13A)-Si(1A)-C(15A)-C(18A)	60.51(13)
C(15A)-Si(1A)-O(5A)-C(10A)	172.39(10)	O(5A)-Si(1A)-C(15A)-C(17A)	-61.71(11)
C(11A)-C(1A)-C(2A)-C(3A)	-130.35(12)	C(14A)-Si(1A)-C(15A)-C(17A)	57.51(12)
C(12A)-C(1A)-C(2A)-C(3A)	101.68(11)	C(13A)-Si(1A)-C(15A)-C(17A)	-179.59(10)
C(4A)-C(1A)-C(2A)-C(3A)	-11.79(9)	C(13B)-Si(1B)-O(5B)-C(10B)	143.52(10)
C(1A)-C(2A)-C(3A)-C(8A)	118.96(11)	C(14B)-Si(1B)-O(5B)-C(10B)	23.03(12)
C(1A)-C(2A)-C(3A)-C(4A)	11.90(9)	C(15B)-Si(1B)-O(5B)-C(10B)	-98.45(11)
C(7A)-O(3A)-C(4A)-C(5A)	-119.54(11)	C(11B)-C(1B)-C(2B)-C(3B)	-132.76(12)
C(7A)-O(3A)-C(4A)-C(3A)	9.46(13)	C(12B)-C(1B)-C(2B)-C(3B)	99.48(12)
C(7A)-O(3A)-C(4A)-C(1A)	105.62(12)	C(4B)-C(1B)-C(2B)-C(3B)	-13.10(10)
C(8A)-C(3A)-C(4A)-O(3A)	-16.92(13)	C(1B)-C(2B)-C(3B)-C(8B)	121.32(12)
C(2A)-C(3A)-C(4A)-O(3A)	99.61(10)	C(1B)-C(2B)-C(3B)-C(4B)	13.26(10)
C(8A)-C(3A)-C(4A)-C(5A)	104.55(13)	C(7B)-O(3B)-C(4B)-C(5B)	-110.85(11)
C(2A)-C(3A)-C(4A)-C(5A)	-138.92(12)	C(7B)-O(3B)-C(4B)-C(3B)	17.60(13)
C(8A)-C(3A)-C(4A)-C(1A)	-128.35(10)	C(7B)-O(3B)-C(4B)-C(1B)	113.37(12)
C(2A)-C(3A)-C(4A)-C(1A)	-11.82(9)	C(8B)-C(3B)-C(4B)-O(3B)	-18.73(13)
C(11A)-C(1A)-C(4A)-O(3A)	24.56(15)	C(2B)-C(3B)-C(4B)-O(3B)	98.87(10)
C(12A)-C(1A)-C(4A)-O(3A)	153.88(11)	C(8B)-C(3B)-C(4B)-C(5B)	100.94(13)
C(2A)-C(1A)-C(4A)-O(3A)	-93.92(11)	C(2B)-C(3B)-C(4B)-C(5B)	-141.46(12)
C(11A)-C(1A)-C(4A)-C(5A)	-103.51(14)	C(8B)-C(3B)-C(4B)-C(1B)	-130.81(11)
C(12A)-C(1A)-C(4A)-C(5A)	25.81(16)	C(2B)-C(3B)-C(4B)-C(1B)	-13.21(10)
C(2A)-C(1A)-C(4A)-C(5A)	138.01(12)	C(11B)-C(1B)-C(4B)-O(3B)	27.06(16)
C(11A)-C(1A)-C(4A)-C(3A)	130.29(12)	C(12B)-C(1B)-C(4B)-O(3B)	157.25(11)
C(12A)-C(1A)-C(4A)-C(3A)	-100.39(12)	C(2B)-C(1B)-C(4B)-O(3B)	-91.69(11)
C(2A)-C(1A)-C(4A)-C(3A)	11.81(10)	C(11B)-C(1B)-C(4B)-C(5B)	-101.06(15)
O(3A)-C(4A)-C(5A)-O(1A)	63.03(12)	C(12B)-C(1B)-C(4B)-C(5B)	29.12(17)
C(3A)-C(4A)-C(5A)-O(1A)	-56.61(14)	C(2B)-C(1B)-C(4B)-C(5B)	140.19(12)
C(1A)-C(4A)-C(5A)-O(1A)	-167.85(10)	C(11B)-C(1B)-C(4B)-C(3B)	131.91(12)
O(3A)-C(4A)-C(5A)-C(6A)	-57.71(13)	C(12B)-C(1B)-C(4B)-C(3B)	-97.90(12)
C(3A)-C(4A)-C(5A)-C(6A)	-177.35(11)	C(2B)-C(1B)-C(4B)-C(3B)	13.16(10)
C(1A)-C(4A)-C(5A)-C(6A)	71.41(15)	O(3B)-C(4B)-C(5B)-O(1B)	64.84(12)
O(1A)-C(5A)-C(6A)-O(2A)	61.22(14)	C(3B)-C(4B)-C(5B)-O(1B)	-53.13(15)
C(4A)-C(5A)-C(6A)-O(2A)	-177.61(11)	C(1B)-C(4B)-C(5B)-O(1B)	-165.20(11)
C(4A)-O(3A)-C(7A)-O(4A)	-179.10(13)	O(3B)-C(4B)-C(5B)-C(6B)	-56.42(13)
C(4A)-O(3A)-C(7A)-C(8A)	2.01(15)	C(3B)-C(4B)-C(5B)-C(6B)	-174.40(11)
O(4A)-C(7A)-C(8A)-C(3A)	168.54(15)	C(1B)-C(4B)-C(5B)-C(6B)	73.54(15)
O(3A)-C(7A)-C(8A)-C(3A)	-12.66(14)	O(1B)-C(5B)-C(6B)-O(2B)	69.72(13)
O(4A)-C(7A)-C(8A)-C(9A)	-67.18(19)	C(4B)-C(5B)-C(6B)-O(2B)	-169.84(10)
O(3A)-C(7A)-C(8A)-C(9A)	111.62(12)	C(4B)-O(3B)-C(7B)-O(4B)	171.68(12)
C(4A)-C(3A)-C(8A)-C(7A)	17.55(13)	C(4B)-O(3B)-C(7B)-C(8B)	-9.65(14)
C(2A)-C(3A)-C(8A)-C(7A)	-78.59(13)	O(4B)-C(7B)-C(8B)-C(3B)	175.69(13)
C(4A)-C(3A)-C(8A)-C(9A)	-101.38(12)	O(3B)-C(7B)-C(8B)-C(3B)	-2.88(14)
C(2A)-C(3A)-C(8A)-C(9A)	162.48(11)	O(4B)-C(7B)-C(8B)-C(9B)	-59.05(18)
C(7A)-C(8A)-C(9A)-C(10A)	173.47(11)	O(3B)-C(7B)-C(8B)-C(9B)	122.39(12)
C(3A)-C(8A)-C(9A)-C(10A)	-70.95(14)	C(4B)-C(3B)-C(8B)-C(7B)	13.34(13)
Si(1A)-O(5A)-C(10A)-C(9A)	137.68(9)	C(2B)-C(3B)-C(8B)-C(7B)	-83.79(13)
C(8A)-C(9A)-C(10A)-O(5A)	-65.95(14)	C(4B)-C(3B)-C(8B)-C(9B)	-109.14(12)
O(5A)-Si(1A)-C(15A)-C(16A)	57.52(12)	C(2B)-C(3B)-C(8B)-C(9B)	153.73(11)
C(14A)-Si(1A)-C(15A)-C(16A)	176.74(11)	C(7B)-C(8B)-C(9B)-C(10B)	173.24(11)
C(13A)-Si(1A)-C(15A)-C(16A)	-60.36(12)	C(3B)-C(8B)-C(9B)-C(10B)	-69.29(14)
O(5A)-Si(1A)-C(15A)-C(18A)	178.39(11)	Si(1B)-O(5B)-C(10B)-C(9B)	166.79(8)

C(8B)-C(9B)-C(10B)-O(5B)	-61.05(14)	C(13B)-Si(1B)-C(15B)-C(17B)	175.20(10)
O(5B)-Si(1B)-C(15B)-C(16B)	-58.91(11)	C(14B)-Si(1B)-C(15B)-C(17B)	-61.31(12)
C(13B)-Si(1B)-C(15B)-C(16B)	56.36(12)	O(5B)-Si(1B)-C(15B)-C(18B)	-179.59(9)
C(14B)-Si(1B)-C(15B)-C(16B)	179.85(10)	C(13B)-Si(1B)-C(15B)-C(18B)	-64.33(12)
O(5B)-Si(1B)-C(15B)-C(17B)	59.94(11)	C(14B)-Si(1B)-C(15B)-C(18B)	59.17(12)

Table S7. Hydrogen bonds for 18a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1A)-H(1A)...O(2B)#1	0.841(19)	1.858(19)	2.6918(14)	170.7(17)
O(2A)-H(2A)...O(1A)#1	0.840(19)	1.953(19)	2.7649(14)	162.5(18)
O(1B)-H(1B)...O(2A)#1	0.945(19)	1.89(2)	2.8166(15)	167.5(16)
O(2B)-H(2B)...O(4B)#2	0.800(19)	1.995(19)	2.7938(14)	175.8(19)

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

PLATON

```
Nr Typ Res Donor --- H....Acceptor [    ARU  ]      D - H      H...A      D...A  D - H...A
A..H..A* A'..H..A" Sum(XY,YZ)  Sum(XZ)
-------------------------------------------------------------------------------------------------
-------------------------------------
 1       1 O1A   -- H1A   .. O2B   [  2565.02]     0.8367     1.8634     2.6922     170.54
 2       2 O1B   -- H1B   .. O2A   [  2565.01]     0.9396     1.8904     2.8167     168.22
 3       1 O2A   -- H2A   .. O1A   [  2555.01]     0.8349     1.9583     2.7652     162.26
 4       2 O2B   -- H2B   .. O4B   [  2565.02]     0.8027     1.9923     2.7936     175.87

 5       2 C3B   -- H3B   .. O4A   [  1565.01]     1.0000     2.2456     3.1540     150.40
 6 Intra 1 C9A   -- H9A1  .. O1A   [          ]     0.9900     2.4646     3.2883     140.37
 7       1 C5A   -- H5A   .. O1B   [  2565.02]     1.0000     2.4889     3.2198     129.59
 8 Intra 2 C8B   -- H8B   .. O5B   [          ]     1.0000     2.5609     2.9397     102.22
 9       1 C10A  -- H10A  .. O4B   [          ]     0.9900     2.5860     3.5282     159.02
10 Intra 2 C9B   -- H9B1  .. O1B   [          ]     0.9900     2.5764     3.3486     134.82
11 Intra 1 C11A  -- H11C  .. O3A   [          ]     0.9800     2.4327     2.8158     102.73

Translation of ARU-code to Equivalent Position Code
===================================================
   [  2555. ]  = -x,-y,-z
   [  2565. ]  = -x,1-y,-z
   [  1565. ]  = x,1+y,z
```