Supporting Information for

Creation of an HDAC-Based Yeast Screening Method for Evaluation of Marine-Derived Actinomycetes: Discovery of Streptosetin A

Part 1

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Part 1

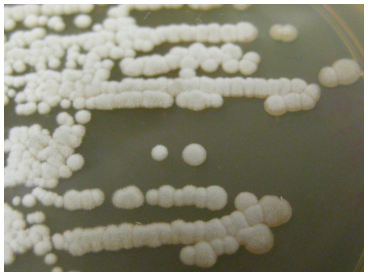


Figure S1. The strain CP13-10 on an ISP2 plate

3'-GCTCAGGACGAACGCTGGCGGCGTGCTTAACACATGCAAGTCGAACGATGAACCGGTTTC
GGCCGGGGATTAGTGGCGAACGGGTGAGTAACACGTGGGCAATCTGCCCTGCACTCTGGG
ACAAGCCCTGGAAACGGGGTCTAATACCGGATATGACACGCTCCCGCATGGGATGCGTGT
GGAAAGCTCCGGCGGTGCAGGATGAGCCCGCGGCCTATCAGCTTGTTGGTGGGGTGATGG
CCTACCAAGGCGACGACGGGTAGCCGGCCTGAGAGGGCGACCGGCCACACTGGGACTGAG
ACACGGCCCAGACTCCTACGGGAGGCAGCAGTGGGGAATATTGCACAATGGGCGAAAGCC
TGATGCAGCGACGCCGCGTGAGGGATGACGGCCTTCGGGTTGTAAACCTCTTTCAGCAGG
GAAGAAGCGAGAGTGACGGTACCTGCAGAAGAAGCGCCGGCTAACTACGTGCCAGCAGCC
GCGGTAATACGTAGGGCGCAAGCGTTGTCCGGAATTATTGGGCGTAAAGAGCTCGTAGGC
GGCTTGTCACGTCGGATGTGAAAGCCCGGGGCTTAACTCCGGGTCTGCATTCGATACGGG
CAGGCTAGAGTTCGGTAGGGGAGATCGGAATTCCTGGTGTAGCGGTGAAATGCGCAGATA
TCAGGAGGAACACCGGTGGCGAAGGCGGATCTCTGGGCCGATACTGACGCTGAGGAGCGA
AAGCGTGGGGAGCGAACAGGATTAGATACCCTGGTAGTCCACGCCGTAAACGTTGGGAAC
TAGGTGTGGGCGACATTCCACGTCGTCCGCGCCGCAGCTAACGCATTAAGTTCCCCGCCT
GGGGAGTACGGCCGCAAGGCTAAAACTCAAAGGAATTGACGGGGGCCCGCACAAGCGGCG
GAGCATGTGGCTTAATTCGACGCAACGCGAAGAACCTTACCAAGGCTTGACATACACCGG
AAACCTCTGGAGACAGGGGCCCCCTTGTGGTCGGTGTACAGGTGGTGCATGGCTGTCGTC
AGCTCGTGTCGTGAGATGTTGGGTTAAGTCCCGCAACGAGCGCAACCCTTGTTCTGTGTT
GCCAGCATGCCTTTCGGGGTGATGGGGACTCACAGGAGACTGCCGGGGTCAACTCGGAGG
AAGGTGGGGACGACGTCAAGTCATCATGCCCCTTATGTCTTGGGCTGCACACGTGCTACA
ATGGCCGGTACAATGAGCTGCGAAGCCGTGAGGTGGAGCGAATCTCAAAAAGCCGGTCTC
AGTTCGGATTGGGGTCTGCAACTCGACCCCATGAAGTCGGAGTCGCTAGTAATCGCAGAT
CAGCATTGCTGCGGTGAATACGTTCCCGGGCCTTGTACACACCGCCCGTCACGTCACGAA
AGTCGGTAACACCCGAAGCCGGTGGCCCAACCCTTGTGGGGGGAGCCGTCGAAGGTGGGA
CTGGCGATTGGGACGAAGTCGTAACA-5'

Figure S2. 16s rRNA sequence of the strain CP13-10 (GenBank accession number: JX235443)

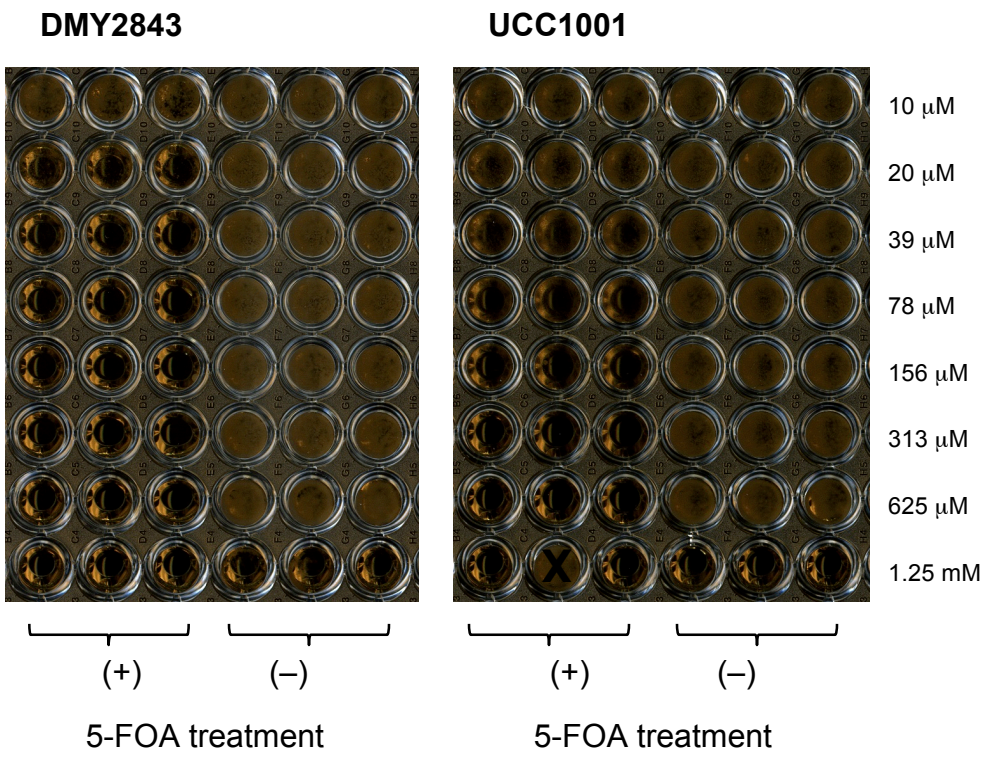


Figure S3. Yeast screening result for splitomicin.

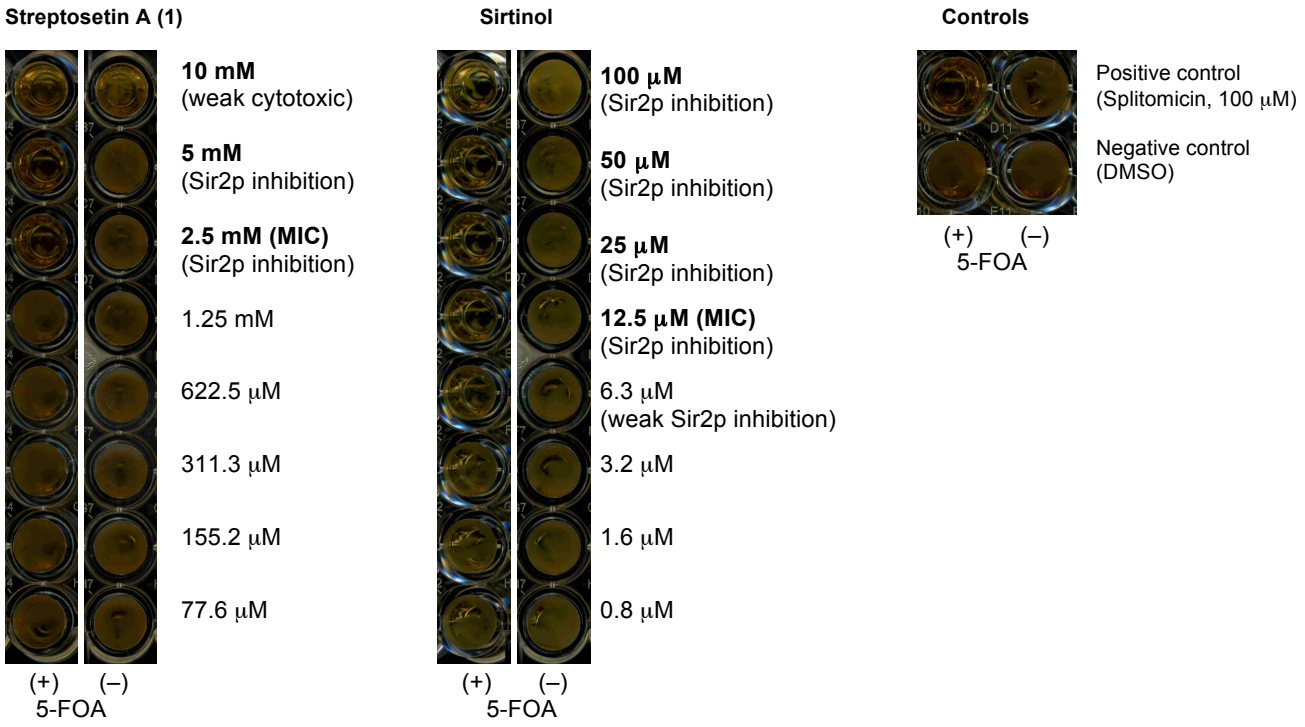


Figure S4. Yeast assay for streptosetin A (**1**) and sirtinol

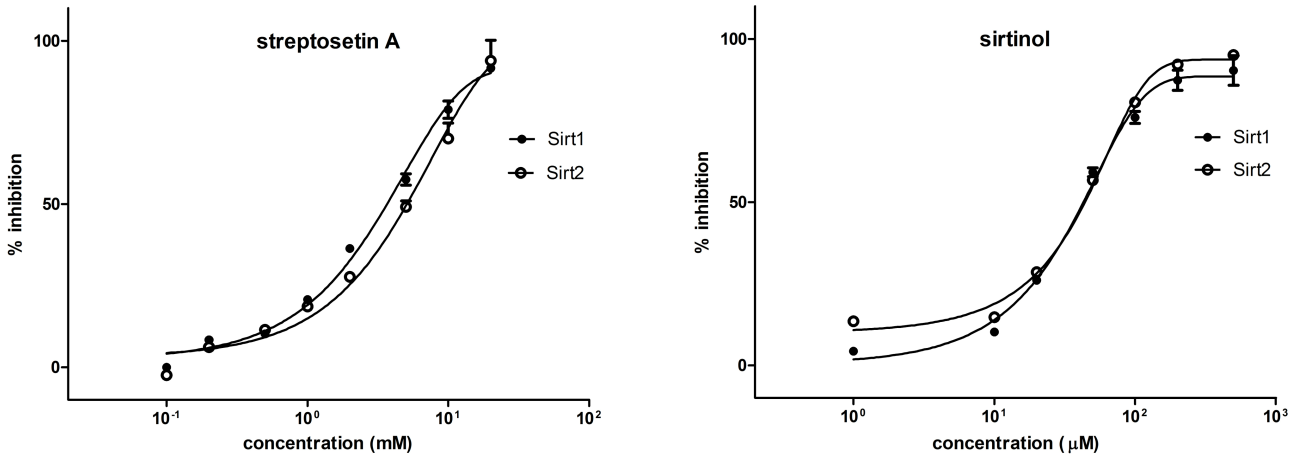
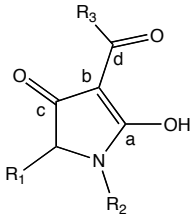


Figure S5. In vitro SIRT1 and SIRT2 assays for streptosetin A (**1**) and sirtinol

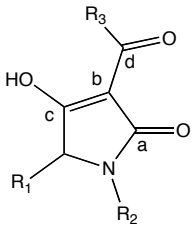
Table S1. Carbon chemical shifts for selected tetramic acid derivatives

Type I tautomer



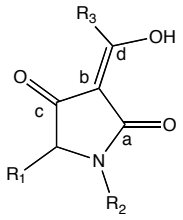
Compound Name	Carbon chemical shift				Solvent	Substituent			X-Ray	Biological source	Ref
	a	b	c	d		R_1	R_2	R_3			
Discodermide	193.5	101.1	178.5	183.9	CD_3OD	CH(OH)alkyl	H	alkyl	N	*Discodermia dissoluta*	1
Epicoccamide A	175.3	101.6	197.6	201.3	CD_3OD	CH_3	CH_3	alkyl	N	*Epicoccum purpurascens*	2
Epicoccamide B	173.1	99.8	192.0	194.6	$CDCl_3$	CH_3	CH_3	alkyl	N	*Pholiota squarrosa*	3
Epicoccamide C	173.1	99.8	192.0	194.5	$CDCl_3$	CH_3	CH_3	alkyl	N		
Epicoccamide D	173.1	99.8	191.9	194.5	$CDCl_3$	CH_3	CH_3	alkyl	N		
Reutericyclin (Major isomer)	167.3	106.1	199.2	195.6	CD_3CN	$CH_2CH(CH_3)_2$	C(=O)alkyl	CH_3	N	*Lactobacillus reuteri* LTH2584	4

Type II tautomer



Compound Name	Carbon chemical shift				Solvent	Substituent			X-Ray	Biological source	Ref
	a	b	c	d		R_1	R_2	R_3			
Altermide A	180.1	103.1	184.8	194.9	CD_3OD	CH_3	CH_3	alkyl	N	*Alteromonas* sp.	5
Altersetin	179.8	99.7	191.5	198.6	DMSO-d_6	$CH(OH)CH_3$	H	decalin	N	*Alternaria* spp.	6
BU-4514N	179.1	104.2	193.2	204.1	CD_3OD/D_2O /4N DCl	None	H	decalin	N	*Microtetraspora* sp.	7
CJ-17572	177.0	100.6	192.3	200.3	$CDCl_3$	$CH(OH)CH_3$	CH_3	decalin	N	*Pezicula* sp.	8
Delaminomycin A	181.5	101.3	192.9	204.8	CD_3OD	OH	H	decalin	N	*Streptomyces albulus* MJ202-72F3	9
Erythroskyrin	173.7	100.8	194.3	172.0	$CDCl_3$	$CH(CH_3)_2$	CH_3	alkyl	N	*Penicillium islandicum*	10
Fuligorubin A	174.1	100.9	174.1	194.5	Acetone-d_6	C_2H_4COOH	CH_3	alkyl	N	*Fuligo septica*	11
Integramycin	177.1	103.3	196.3	192.3	Pyridine-d_5	OH	H	decalin	N	*Actinoplanes* sp.	12
	176.4	102.6	194.3	192.2	Acetone-d_6						
Lydicamycin	181.0	103.0	192.3	204.0	CD_3OD	None	H	decalin	N	*Streptomyces lydicus*	13
Oxasetin	166.5	106.3	164.2	200.2	DMSO-d_6	=O	H	decalin	N	*Vaginatispora aquatic* HK1821	14
Pachydermin	165.7	99.4	177.0	179.3	DMSO-d_6	=CHPh(OH)Cl	H	COOH	N	*Chamonixia pachydermis*	15
Reutericyclin (Minor isomer)	174.8	103.6	194.5	189.3	CD_3CN	$CH_2CH(CH_3)_2$	C(=O)alkyl	CH_3	N	*Lactobacillus reuteri* LTH2584	4
Vergineone	177.1	99.6	193.6	197.5	DMSO-d_6	CH_2PhOH	H	alkyl	N	*Lachnum virgineum*	16

Type III tautomer



Compound Name	Carbon chemical shift				Solvent	Substituent			X-Ray	Biological source	Ref
	a	b	c	d		R_1	R_2	R_3			
Aflastatin A	173.4	98.1	192.6	191.5	DMSO-d_6	CH_3	CH_3	alkyl	N	*Aspergillus parasiticus*	17
Aflastatin B	ND	ND	196.1	195.7	DMSO-d_6	CH_3	H	alkyl	N		
Ancorinoside A	174.3	101.8	194.1	191.4	Pyridine-d_5	CH_2COOH	CH_3	alkyl	N	*Ancorina* sp.	18
Aurantoside A	174.8	102.0	195.0	176.1	CD_3OD	CH_2CONH_2	Sugars	alkyl	N	*Theonella* sp.	19
Aurantoside B	174.9	102.0	195.1	176.2	CD_3OD	CH_2CONH_2	Sugars	alkyl	N		
Aurantoside D	176.2	102.0	194.9	174.8	CD_3OD	CH_2CONH_2	Sugars	alkyl	N	*Siliquariaspongia japonica*	20
Blasticidin A	174.4	99.7	189.4	191.2	DMSO-d_6	None	CH_3	alkyl	N	*Aspergillus parasiticus*	21
Cissetin	177.6	98.1	191.4	201.8	$CDCl_3$	$CH(OH)CH_3$	CH_3	decalin	N	An unidentified fungus	22
CJ-21058	178.1	101.6	191.4	197.7	CD_3CN	$CH(OH)CH_3$	CH_3	decalin	N	An unidentified fungus	23
Coniosetin	179.5	99.5	191.1	198.2	DMSO-d_6	$CH(OH)CH_3$	CH_3	decalin	N	*Coniochaeta ellipsoidea*	24
	181.5	101.5	193.5	201.3	CD_3OD						
Epicoccarine A	175.3	100.4	193.7	193.9	$CDCl_3$	CH_2PhOH	H	alkyl	N	*Pholiota squarrosa*	25
Equisetin	176.7	99.8	198.9	190.6	CD_3CN	CH_2OH	CH_3	decalin	N	*Fusarium equiseti Fusarium heterosporum*	26
Harzianic acid	173.9	100.9	198.9	175.9	CD_3OD	alkyl	CH_3	alkyl	N	*Trichoderma harzianum*	27
Macrocidin	176.8	103.5	197.5	193.1	CD_3OD	alkyl	H	alkyl	**Y**	*Phoma macrostoma*	28
Militarinone	175.4	100.4	192.8	172,2	DMSO-d_6	CH(OH)PhOH	H	alkyl	N	*Paecilomyces militaris*	29
Paecilosetin	179.5	100.3	191.6	197.6	DMSO-d_6	$CH(OH)CH_3$	H	decalin	N	*Paecilomyces farinosus*	30
PF1052	173.6	103.9	194.1	190.2	NA	$CH(CH_3)C_2H_5$	CH_3	decalin	N	*Phoma* sp.	31
Polycephalin B	175.1	101.4	194.3	173.3	CD_3OD/ $CDCl_3$	CH_2OH	CH_3	alkyl	N	*Physarum polycephalum*	32
Phomasetin	178.0	101.6	191.5	197.5	CD_3CN	CH_2OH	CH_3	decalin	N	*Phoma* sp.	26
Ravenic acid	176.6	99.7	192.4	174.8	$CDCl_3$	None	H	alkyl	N	*Penicillium* sp.	33
Reutericyclin (Minor isomer)	174.8	103.6	194.5	189.3	CD_3CN	$CH_2CH(CH_3)_2$	C(=O)alkyl	CH_3	N	*Lactobacillus reuteri* LTH2584	4
Tirandalydigin*	179.9	99.7	193.5	186.1	CD_3OD	None	H	alkyl	N	*Streptomyces* sp. AB-1006A-9	34
Tirandamycin	174.7*	100.0	192.4	176.4*	$CDCl_3$	None	H	alkyl	N	*Streptomyces tirandis*	35
Xanthobaccin A*	180.1	102.9	194.5	183.3	CD_3OD	CH(OH)alkyl	H	alkyl	N	*Strenotrophomonas* sp.	36

Table S2. Crystal data and structure refinement for **1**

Empirical formula	$C_{20}H_{28}Cl_3NO_6$
Formula weight	484.78
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Trigonal
Space group	$P3_221$
Unit cell dimensions	a = 11.1313(3) Å α = 90°
	b = 11.1313(3) Å β = 90°
	c = 33.9045(9) Å γ = 120°
Volume	3638.14(17) Å^3
Z	6
Density (calculated)	1.328 g.cm^{-3}
Absorption coefficient (μ)	3.716 mm^{-1}
F(000)	152
Crystal size	0.51 × 0.22 × 0.13 mm^3
θ range for data collection	3.91 to 67.96°
Index ranges	-12 ≤ h ≤ 13, -13 ≤ k ≤ 13, -40 ≤ l ≤ 40
Reflections collected	19805
Independent reflections	4334 [R_{int} = 0.0353]
Completeness to θ = 67.96°	99.1 %
Absorption correction	numerical
Max. and min. transmission	0.8361 and 0.4396
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4334 / 0 / 297
Goodness-of-fit on F^2	1.023
Final R indices [I>2σ(I)]	R_1 = 0.0942, wR_2 = 0.2665
R indices (all data)	R_1 = 0.1032, wR_2 = 0.2793
Absolute structure parameter	0.06(6)
Largest diff. peak and hole	0.612 and -0.800 e$^-$. Å^{-3}

Table S3. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **1**

	x	y	z	U(eq)
O(1)	0.5253(6)	0.0530(4)	0.29296(10)	0.062(1)
O(3)	0.6174(5)	0.0952(3)	0.22431(9)	0.053(1)
O(9)	0.9036(3)	0.2843(4)	0.05550(8)	0.042(1)
O(11)	0.6309(4)	0.2684(5)	0.06889(10)	0.060(1)
O(18)	0.6308(6)	0.4970(4)	0.24808(10)	0.067(1)
N(1)	0.5251(8)	0.2389(5)	0.32084(12)	0.070(2)
C(1)	0.5490(8)	0.1801(6)	0.29103(14)	0.056(2)
C(2)	0.6045(8)	0.2694(5)	0.25746(14)	0.055(2)
C(3)	0.6395(7)	0.2168(5)	0.22347(13)	0.049(1)
C(4)	0.7067(6)	0.3050(5)	0.18597(12)	0.040(1)
C(5)	0.7598(6)	0.2280(5)	0.15921(12)	0.039(1)
C(6)	0.8845(7)	0.2242(6)	0.17593(13)	0.047(1)
C(7)	0.9443(6)	0.1642(5)	0.14794(15)	0.046(1)
C(8)	0.9192(6)	0.1528(5)	0.10874(13)	0.046(1)
C(9)	0.8343(5)	0.2053(5)	0.08960(12)	0.040(1)
C(10)	0.7983(5)	0.2922(4)	0.11711(12)	0.034(1)
C(11)	0.6859(5)	0.3154(5)	0.10010(12)	0.041(1)
C(12)	0.6445(6)	0.3979(5)	0.12631(13)	0.043(1)
C(13)	0.5890(6)	0.3183(5)	0.16551(13)	0.040(1)
C(14)	0.4572(6)	0.1788(5)	0.15889(15)	0.049(1)
C(15)	0.3361(8)	0.1912(8)	0.1409(2)	0.075(2)
C(16)	0.8277(6)	0.4499(5)	0.19766(13)	0.046(1)
C(17)	0.9726(8)	0.0819(8)	0.08205(18)	0.068(2)
C(18)	0.6057(9)	0.3943(6)	0.26746(14)	0.063(2)
C(19)	0.5564(10)	0.3781(7)	0.31071(17)	0.077(3)
C(1S)	0.196(2)	0.299(3)	0.2778(6)	0.110(7)
Cl(1)	0.1900(6)	0.1663(7)	0.31660(18)	0.129(2)
Cl(2)	0.2484(5)	0.2625(6)	0.23744(17)	0.112(2)
Cl(3)	0.0366(16)	0.3299(9)	0.28282(19)	0.230(7)
C(2S)	0.1078(19)	-0.2876(18)	0.3131(5)	0.084(4)
Cl(4)	-0.0666(6)	-0.4017(7)	0.29598(13)	0.213(3)
Cl(5)	0.1633(5)	-0.1068(6)	0.31312(17)	0.115(2)
O(1W)	-0.1355(17)	0.2253(18)	0.3141(4)	0.118(5)
O(2W)	0.2365(7)	0.4236(7)	0.2944(2)	0.041(2)
H(1A)	0.5340	0.0276	0.2710	0.093
H(9)	0.9756	0.3540	0.0621	0.063
H(1B)	0.4949	0.2005	0.3434	0.084
H(5A)	0.6843	0.1319	0.1564	0.047
H(6A)	0.9555	0.3179	0.1827	0.057
H(6B)	0.8570	0.1697	0.2000	0.057
H(7A)	1.0017	0.1332	0.1580	0.056
H(9A)	0.7471	0.1248	0.0810	0.048
H(10A)	0.8819	0.3835	0.1197	0.041
H(12A)	0.5733	0.4100	0.1136	0.052
H(12B)	0.7240	0.4888	0.1313	0.052
H(13A)	0.5650	0.3741	0.1827	0.048
H(14A)	0.4274	0.1306	0.1839	0.058
H(14B)	0.4787	0.1229	0.1415	0.058
H(15A)	0.2554	0.1007	0.1389	0.112
H(15B)	0.3618	0.2317	0.1151	0.112
H(15C)	0.3161	0.2489	0.1575	0.112

H(16A)	0.7913	0.5087	0.2051	0.069
H(16B)	0.8893	0.4901	0.1756	0.069
H(16C)	0.8774	0.4406	0.2195	0.069
H(17A)	1.0041	0.0311	0.0977	0.102
H(17B)	1.0483	0.1503	0.0666	0.102
H(17C)	0.8995	0.0193	0.0648	0.102
H(19A)	0.6289	0.4464	0.3276	0.093
H(19B)	0.4747	0.3875	0.3130	0.093
H(1SA)	0.2750	0.3876	0.2861	0.132
H(2SA)	0.1764	-0.3091	0.3023	0.100

Table S4. Bond lengths [Å] and angles [°] for **1**

atom-atom	distance	atom-atom	distance
O(1)-C(1)	1.305(6)	O(3)-C(3)	1.249(6)
O(9)-C(9)	1.424(5)	O(11)-C(11)	1.203(6)
O(18)-C(18)	1.224(6)	N(1)-C(1)	1.302(7)
N(1)-C(19)	1.449(7)	C(1)-C(2)	1.433(7)
C(2)-C(18)	1.424(7)	C(2)-C(3)	1.432(7)
C(3)-C(4)	1.551(6)	C(4)-C(16)	1.549(7)
C(4)-C(5)	1.554(7)	C(4)-C(13)	1.554(8)
C(5)-C(6)	1.519(8)	C(5)-C(10)	1.557(5)
C(6)-C(7)	1.495(8)	C(7)-C(8)	1.351(7)
C(8)-C(9)	1.486(8)	C(8)-C(17)	1.504(8)
C(9)-C(10)	1.535(7)	C(10)-C(11)	1.512(7)
C(11)-C(12)	1.506(8)	C(12)-C(13)	1.545(6)
C(13)-C(14)	1.528(7)	C(14)-C(15)	1.547(10)
C(18)-C(19)	1.544(7)	C(1S)-Cl(2)	1.62(3)
C(1S)-Cl(1)	1.957(19)	C(1S)-Cl(3)	1.97(2)
C(2S)-Cl(5)	1.785(19)	C(2S)-Cl(4)	1.804(19)
C(2S)-Cl(4)#1	2.013(19)	Cl(4)-C(2S)#1	2.013(19)
O(1)-H(1A)	0.8200	O(9)-H(9)	0.8200
N(1)-H(1B)	0.8600	C(5)-H(5A)	0.9800
C(6)-H(6A)	0.9700	C(6)-H(6B)	0.9700
C(7)-H(7A)	0.9300	C(9)-H(9A)	0.9800
C(10)-H(10A)	0.9800	C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700	C(13)-H(13A)	0.9800
C(14)-H(14A)	0.9700	C(14)-H(14B)	0.9700
C(15)-H(15A)	0.9600	C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600	C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600	C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600	C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600	C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700	C(1S)-H(1SA)	0.9800
C(2S)-H(2SA)	0.9800		

Symmetry transformations used to generate equivalent atoms:
#1 -x,-x+y,-z+2/3

Table S5. Anisotropic displacement parameters ($Å^2x10^3$) for **1**

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	0.129(4)	0.045(2)	0.0283(16)	0.0086(15)	0.019(2)	0.057(3)
O(3)	0.110(3)	0.0311(17)	0.0298(16)	0.0054(14)	0.0216(19)	0.044(2)
O(9)	0.0303(16)	0.0450(19)	0.0206(13)	0.0005(13)	0.0001(12)	-0.0032(14)
O(11)	0.043(2)	0.089(3)	0.0250(16)	-0.0068(18)	-0.0022(15)	0.016(2)
O(18)	0.146(4)	0.040(2)	0.0316(16)	0.0108(16)	0.025(2)	0.060(3)
N(1)	0.157(6)	0.054(3)	0.0255(19)	0.014(2)	0.033(3)	0.073(4)
C(1)	0.116(5)	0.040(3)	0.024(2)	0.006(2)	0.017(3)	0.047(3)
C(2)	0.120(5)	0.038(3)	0.024(2)	0.007(2)	0.015(3)	0.053(3)
C(3)	0.096(4)	0.032(2)	0.024(2)	0.0066(18)	0.012(2)	0.035(3)
C(4)	0.072(3)	0.023(2)	0.0198(18)	-0.0008(17)	0.005(2)	0.020(2)
C(5)	0.065(3)	0.023(2)	0.0192(19)	0.0001(16)	0.006(2)	0.015(2)
C(6)	0.078(4)	0.039(3)	0.025(2)	0.0006(19)	0.000(2)	0.029(3)
C(7)	0.064(3)	0.038(3)	0.036(2)	0.003(2)	0.004(2)	0.024(2)
C(8)	0.059(3)	0.030(2)	0.032(2)	0.0005(19)	0.012(2)	0.010(2)
C(9)	0.038(2)	0.032(2)	0.0215(19)	-0.0043(18)	0.0024(18)	-0.0044(19)
C(10)	0.039(2)	0.025(2)	0.0231(19)	0.0025(16)	0.0023(17)	0.0037(17)
C(11)	0.040(2)	0.041(3)	0.0194(19)	0.0056(18)	0.0057(18)	0.003(2)
C(12)	0.055(3)	0.031(2)	0.031(2)	0.0071(19)	0.002(2)	0.012(2)
C(13)	0.063(3)	0.027(2)	0.027(2)	-0.0002(17)	0.008(2)	0.021(2)
C(14)	0.067(3)	0.025(2)	0.040(2)	0.0008(19)	0.020(2)	0.012(2)
C(15)	0.057(4)	0.054(4)	0.088(5)	0.008(4)	-0.005(4)	0.009(3)
C(16)	0.076(4)	0.026(2)	0.026(2)	-0.0036(18)	-0.006(2)	0.018(2)
C(17)	0.088(5)	0.073(4)	0.042(3)	-0.004(3)	0.020(3)	0.040(4)
C(18)	0.132(6)	0.048(3)	0.027(2)	0.006(2)	0.016(3)	0.059(4)
C(19)	0.169(8)	0.048(3)	0.038(3)	0.014(3)	0.036(4)	0.072(5)
C(1S)	0.097(13)	0.132(17)	0.106(14)	0.019(12)	-0.051(12)	0.061(12)
Cl(1)	0.090(3)	0.140(5)	0.126(4)	0.075(4)	0.000(3)	0.033(3)
Cl(2)	0.085(3)	0.118(4)	0.116(4)	0.052(3)	0.007(3)	0.037(3)
Cl(3)	0.49(2)	0.143(6)	0.092(4)	0.041(4)	0.056(7)	0.187(10)
Cl(4)	0.207(5)	0.296(7)	0.143(3)	-0.141(4)	-0.088(3)	0.132(5)
Cl(5)	0.078(3)	0.136(4)	0.122(4)	-0.061(4)	-0.027(3)	0.047(3)

Table S6. Torsion angles [°] for **1**

atom-atom-atom-atom	angle	atom-atom-atom-atom	angle	
C(19)-N(1)-C(1)-O(1)	-178.5(8)	C(19)-N(1)-C(1)-C(2)	2.5(10)	N(1)-C(1)-C(2)-
C(18)	-4.2(9)	O(1)-C(1)-C(2)-C(18)	176.8(8)	N(1)-C(1)-C(2)-
C(3)	177.7(7)	O(1)-C(1)-C(2)-C(3)	-1.2(12)	C(18)-C(2)-C(3)-
O(3)	-175.8(9)	C(1)-C(2)-C(3)-O(3)	1.5(10)	C(18)-C(2)-C(3)-
C(4)	5.6(14)	C(1)-C(2)-C(3)-C(4)	-177.1(6)	O(3)-C(3)-C(4)-
C(16)	-132.4(6)	C(2)-C(3)-C(4)-C(16)	46.2(8)	O(3)-C(3)-C(4)-
C(5)	-11.0(8)	C(2)-C(3)-C(4)-C(5)	167.6(6)	O(3)-C(3)-C(4)-
C(13)	108.5(6)	C(2)-C(3)-C(4)-C(13)	-72.9(7)	C(16)-C(4)-C(5)-
C(6)	51.1(5)	C(3)-C(4)-C(5)-C(6)	-70.0(6)	C(13)-C(4)-C(5)-
C(6)	174.3(4)	C(16)-C(4)-C(5)-C(10)	-71.8(5)	C(3)-C(4)-C(5)-
C(10)	167.2(4)	C(13)-C(4)-C(5)-C(10)	51.5(5)	C(4)-C(5)-C(6)-
C(7)	-173.5(4)	C(10)-C(5)-C(6)-C(7)	-48.5(5)	C(5)-C(6)-C(7)-
C(8)	18.4(7)	C(6)-C(7)-C(8)-C(9)	2.9(8)	C(6)-C(7)-C(8)-
C(17)	-175.3(6)	C(7)-C(8)-C(9)-O(9)	132.3(5)	C(17)-C(8)-C(9)-
O(9)	-49.4(6)	C(7)-C(8)-C(9)-C(10)	9.0(7)	C(17)-C(8)-C(9)-
C(10)	-172.7(5)	O(9)-C(9)-C(10)-C(11)	69.8(5)	C(8)-C(9)-C(10)-
C(11)	-166.6(4)	O(9)-C(9)-C(10)-C(5)	-164.5(4)	C(8)-C(9)-C(10)-
C(5)	-40.9(5)	C(6)-C(5)-C(10)-C(11)	-173.4(4)	C(4)-C(5)-C(10)-
C(11)	-47.4(5)	C(6)-C(5)-C(10)-C(9)	60.6(5)	C(4)-C(5)-C(10)-
C(9)	-173.4(4)	C(9)-C(10)-C(11)-O(11)	1.1(6)	C(5)-C(10)-C(11)-
O(11)	-124.6(5)	C(9)-C(10)-C(11)-C(12)	178.9(4)	C(5)-C(10)-C(11)-
C(12)	53.1(5)	O(11)-C(11)-C(12)-C(13)	117.3(5)	C(10)-C(11)-C(12)-
C(13)	-60.5(5)	C(11)-C(12)-C(13)-C(14)	-63.9(6)	C(11)-C(12)-C(13)-
C(4)	61.7(5)	C(16)-C(4)-C(13)-C(14)	-171.1(4)	C(3)-C(4)-C(13)-
C(14)	-52.4(5)	C(5)-C(4)-C(13)-C(14)	65.6(5)	C(16)-C(4)-C(13)-
C(12)	64.5(5)	C(3)-C(4)-C(13)-C(12)	-176.7(4)	C(5)-C(4)-C(13)-
C(12)	-58.7(5)	C(12)-C(13)-C(14)-C(15)	-60.5(6)	C(4)-C(13)-C(14)-
C(15)	176.4(5)	C(1)-C(2)-C(18)-O(18)	-172.2(9)	C(3)-C(2)-C(18)-
O(18)	5.4(17)	C(1)-C(2)-C(18)-C(19)	3.9(9)	C(3)-C(2)-C(18)-
C(19)	-178.5(9)	C(1)-N(1)-C(19)-C(18)	0.1(10)	O(18)-C(18)-C(19)-
N(1)	174.1(8)	C(2)-C(18)-C(19)-N(1)	-2.5(9)	Cl(5)-C(2S)-Cl(4)-
C(2S)#1	-89.0(9)	Cl(4)#1-C(2S)-Cl(4)-C(2S)#1	17.1(11)	

Symmetry transformations used to generate equivalent atoms:

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

Table S7. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for **1**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...O(3)	0.82	1.80	2.491(5)	141.3
O(9)-H(9)...O(18)#2	0.82	1.88	2.696(4)	171.2
N(1)-H(1B)...O(9)#3	0.86	1.96	2.804(6)	165.7
N(1)-H(1B)...O(11)#3	0.86	2.65	3.077(6)	111.7

Symmetry transformations used to generate equivalent atoms:

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

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