Supplementary Information for:

FACILE SYNTHESIS AND X-RAY STRUCTURE OF [1,2,4]TRIAZOLO[4,3-A]PYRIDINES VIA OXIDATIVE CYCLIZATION USING N-CHLOROSUCCINIMIDE (NCS)

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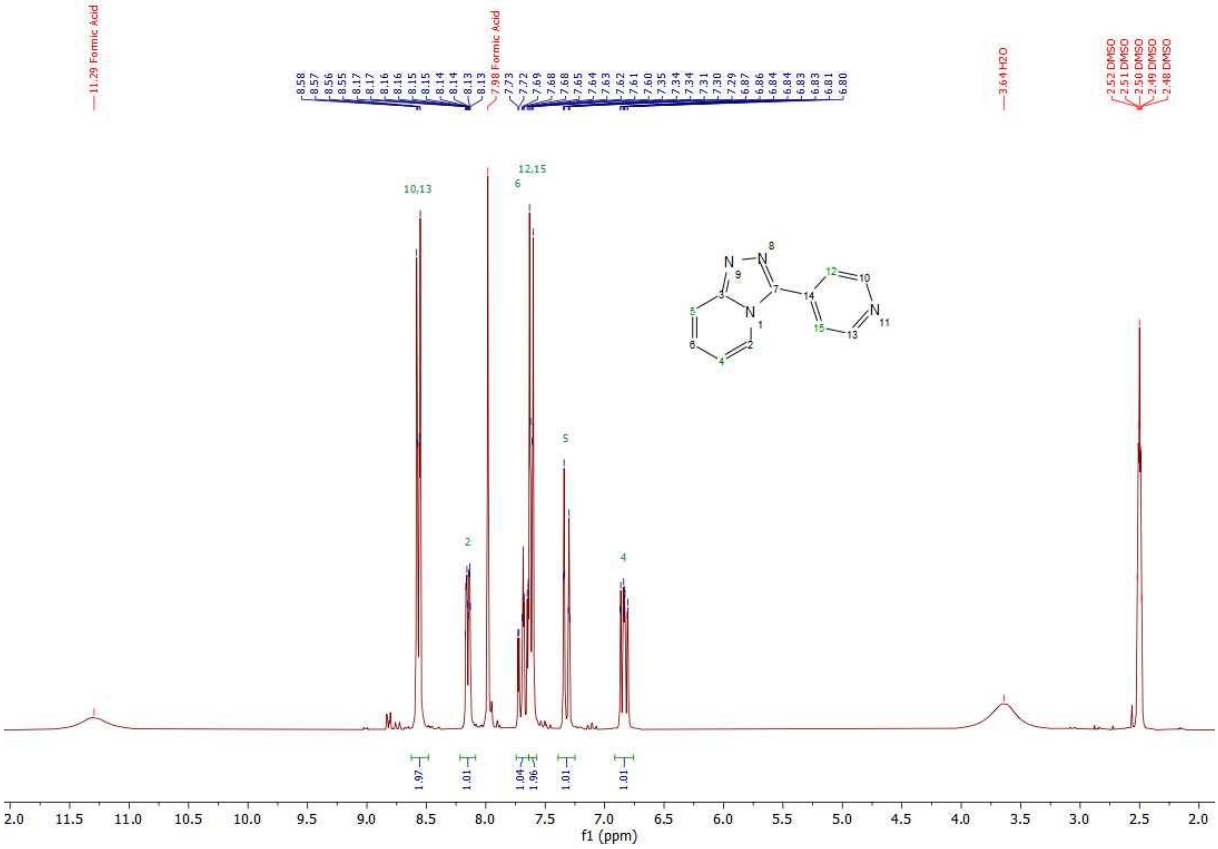

Figure S1. [1]H NNR of **1**.

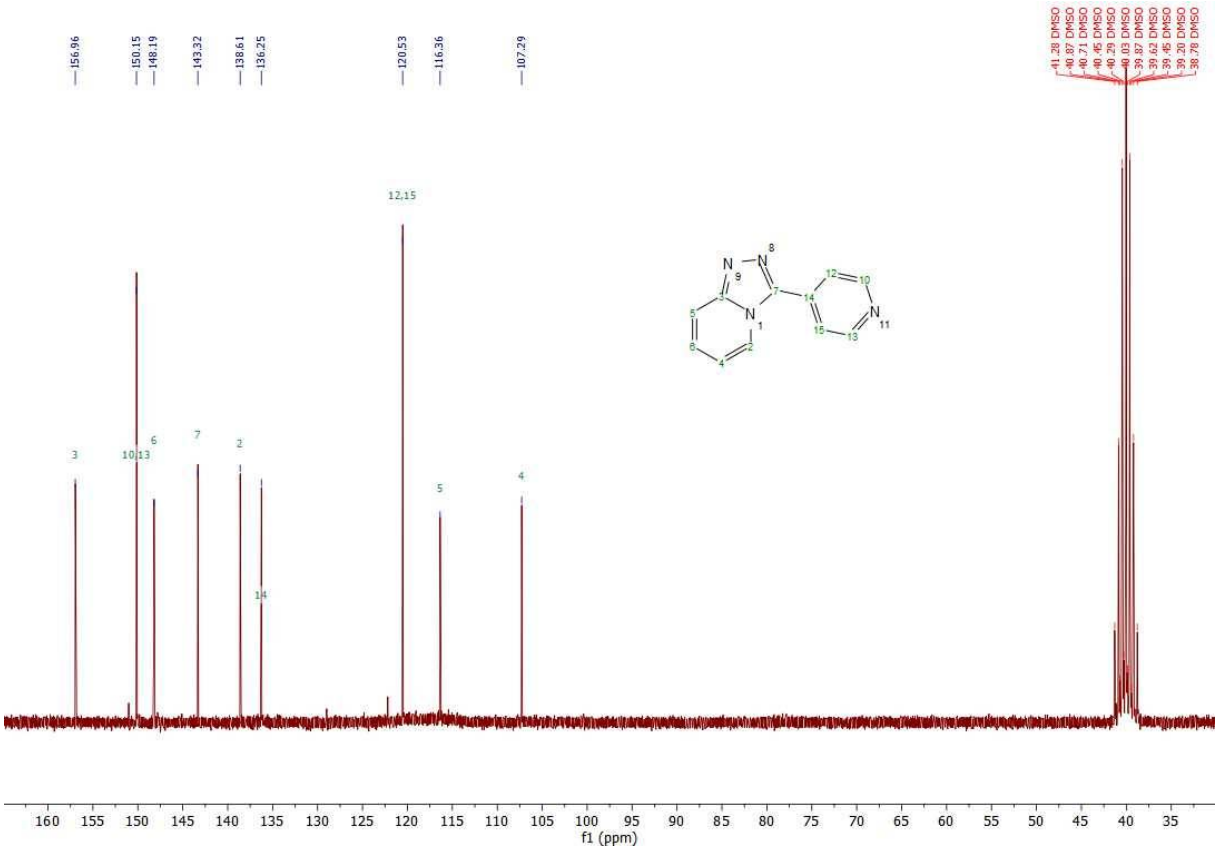

Figure S2. ^{13}C NMR of **1**.

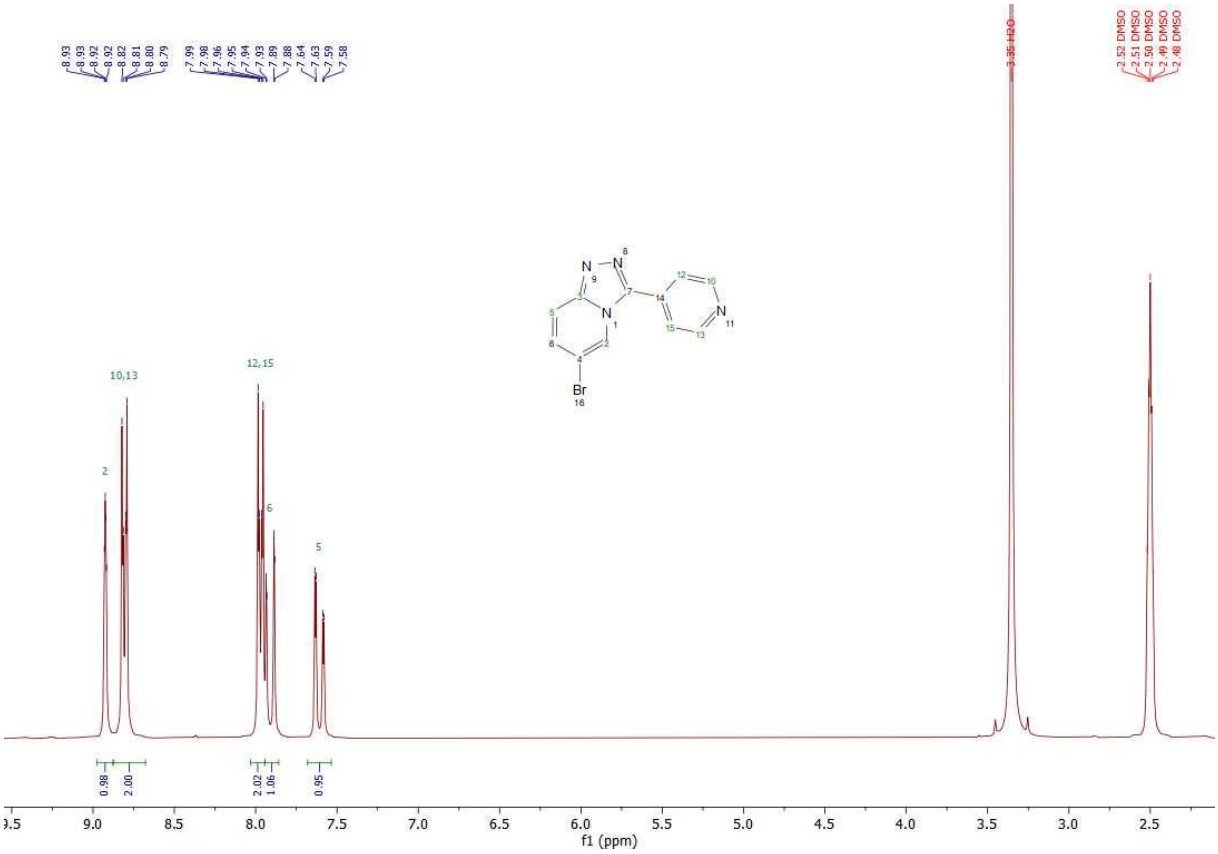

Figure S3. ^{1}H NMR of **2**.

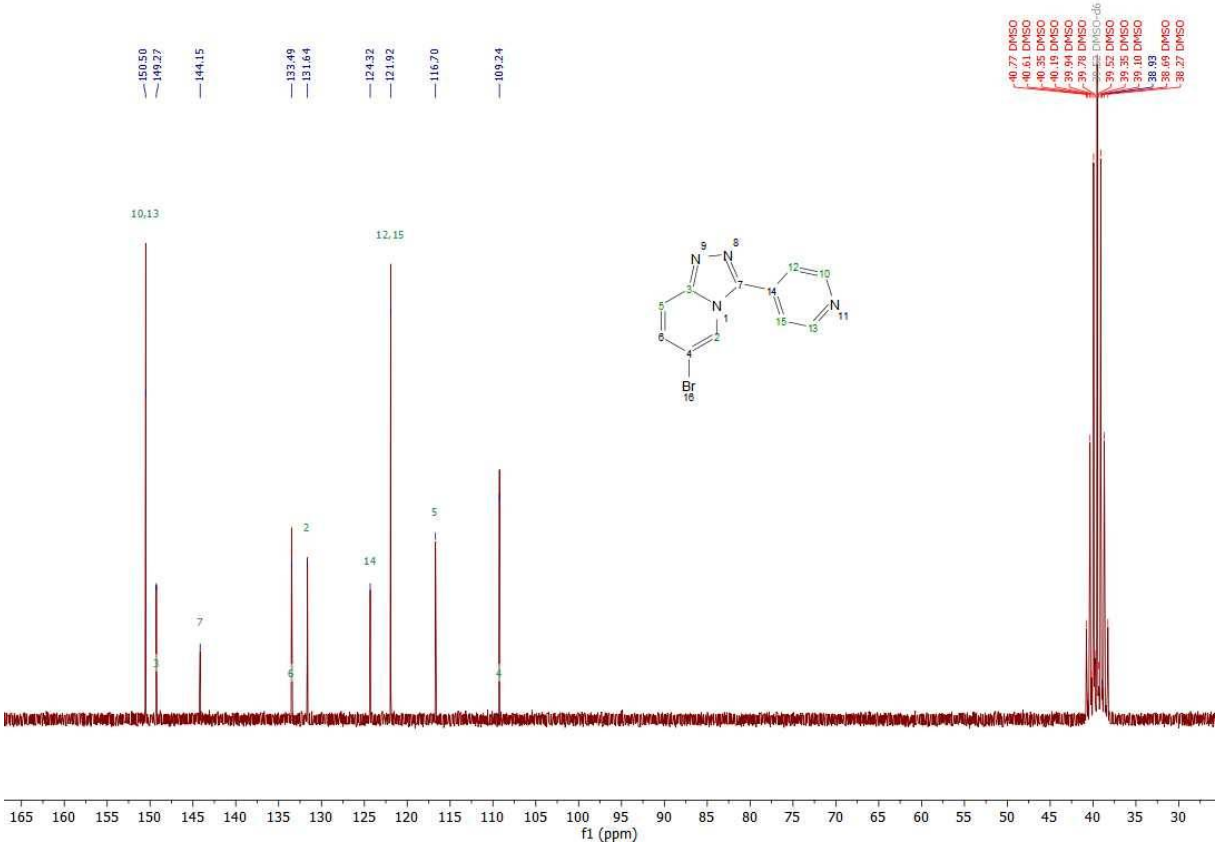

Figure S4. ^{13}C NMR of **2**.

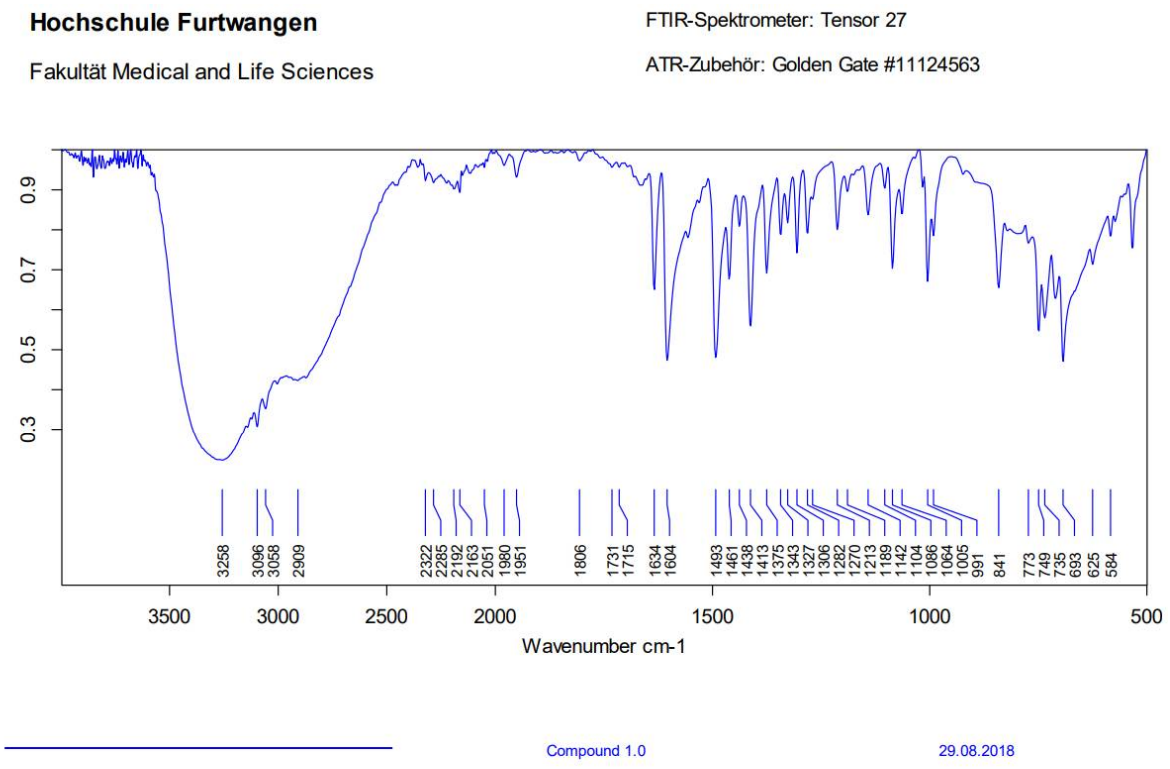

Figure S5. FTIR-Spectrum of **1**.

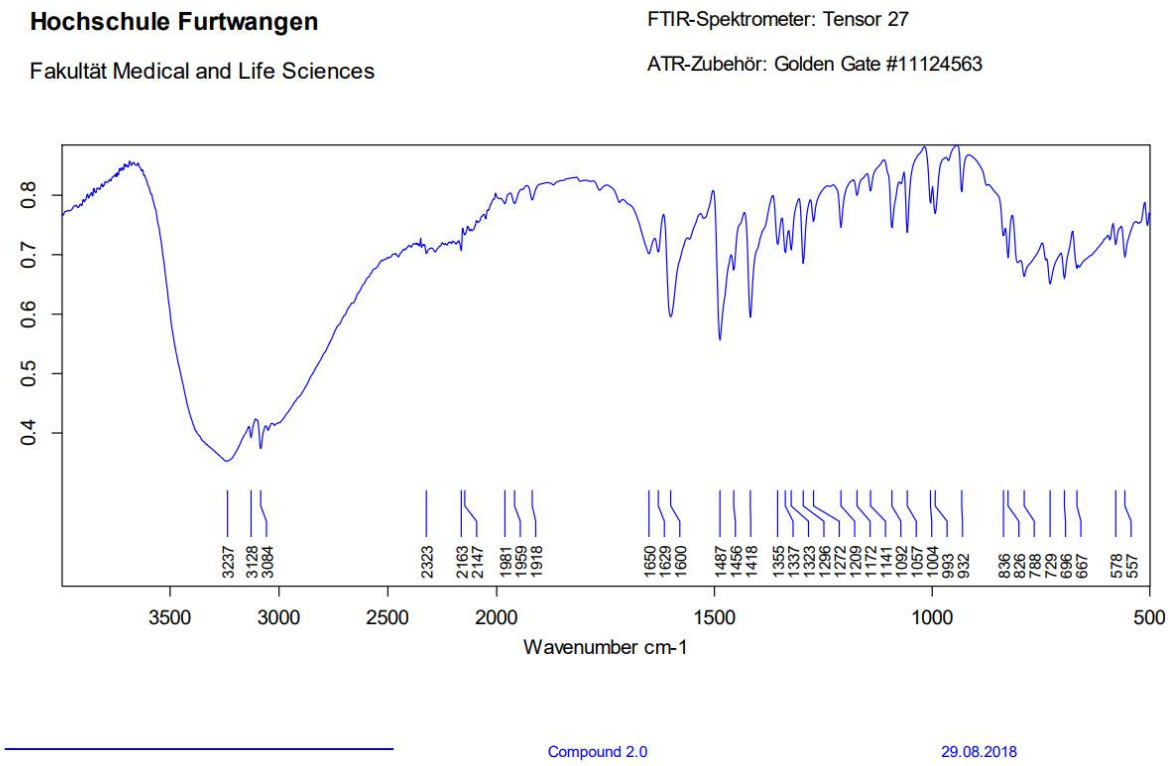

Figure S6. FTIR-Spectrum of **2**.

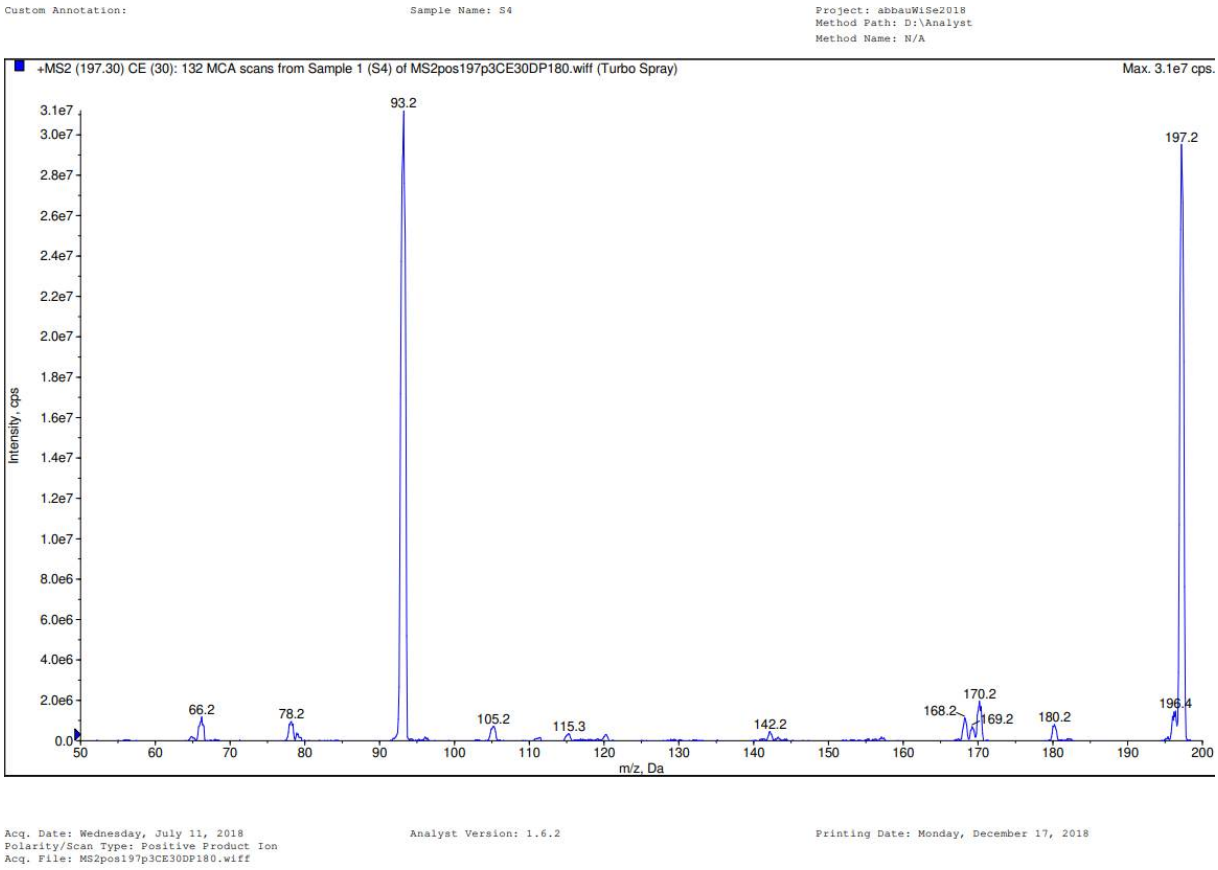

Figure S7. Fragment Ion Scan of **1**.

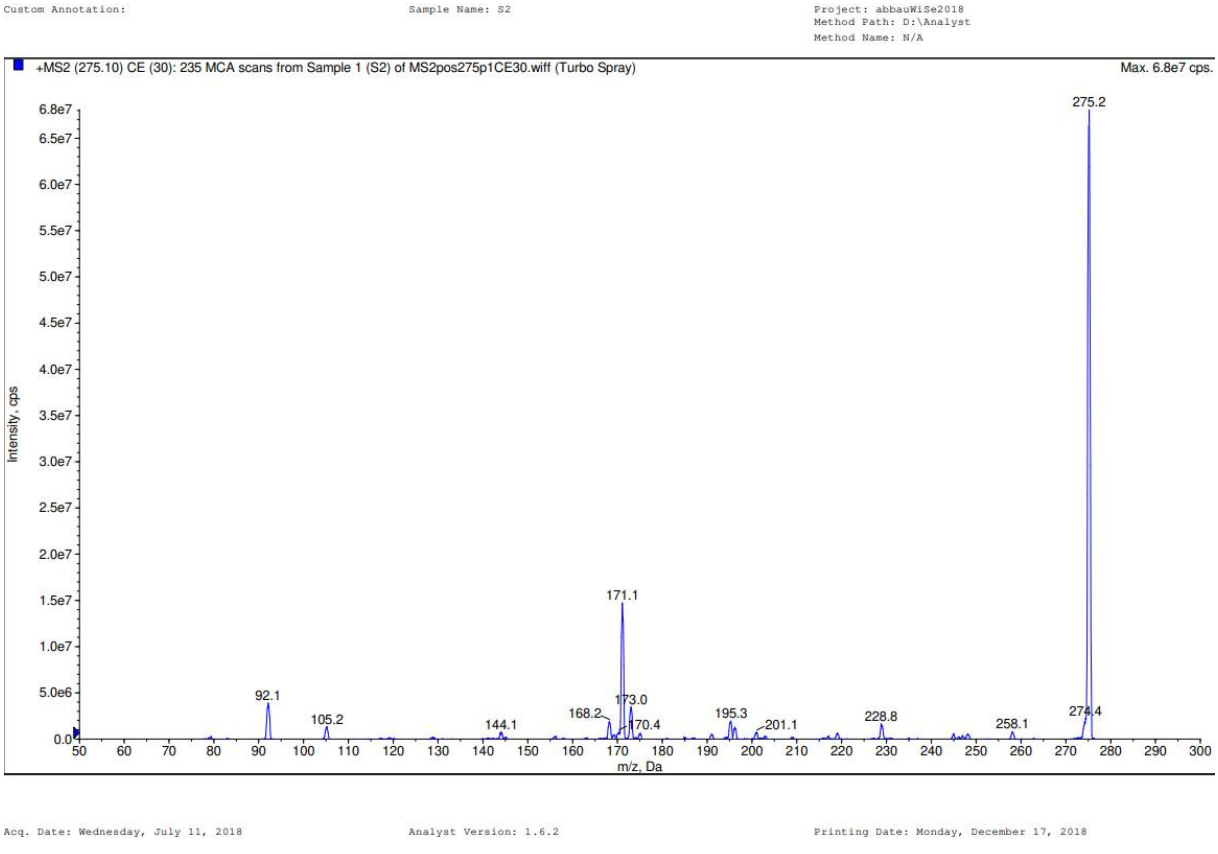

Figure S8. Fragment Ion Scan of **2**.

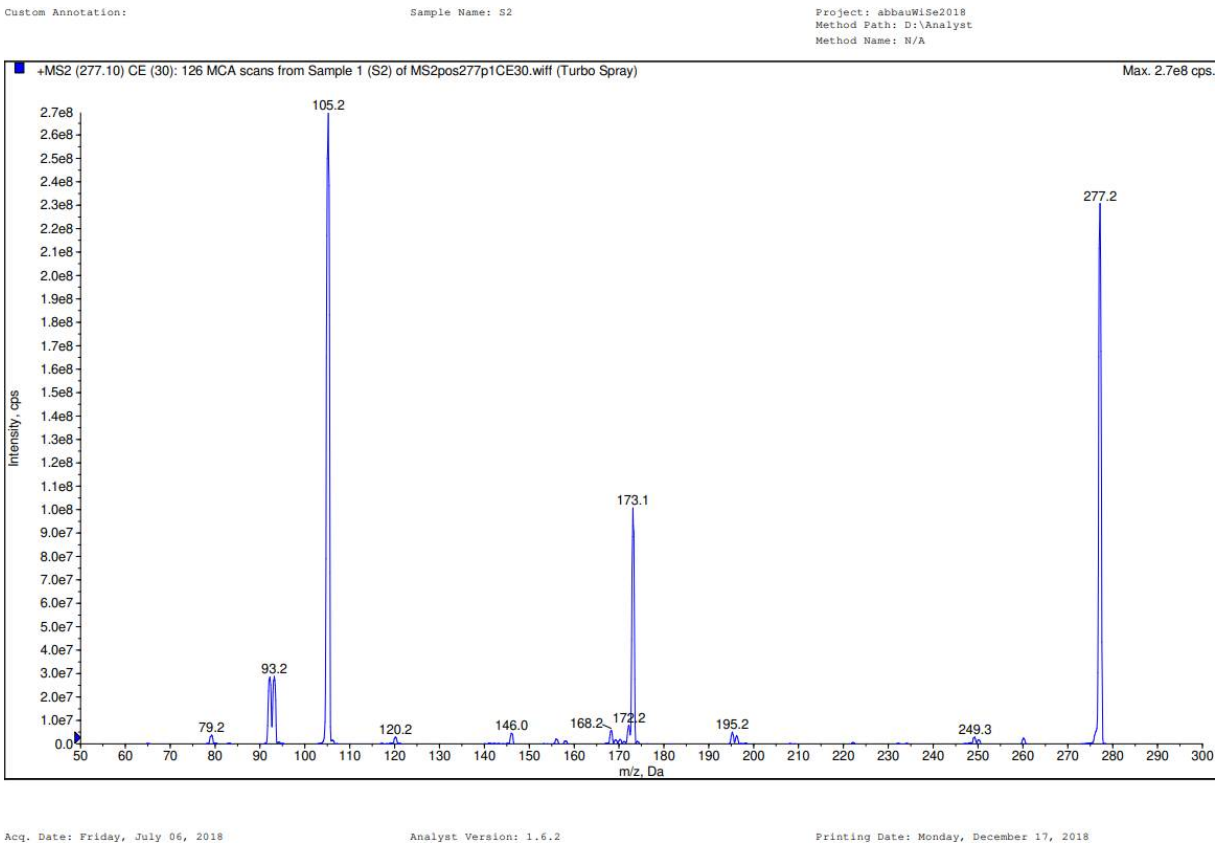

Figure S9. Fragment Ion Scan of **2**.

Table S1. Crystal data and structure refinement for 1

CCDC code	204925
Empirical formula	$C_{11}H_{14}N_4O_3$
moiety formula	$C_{11}H_8N_4$, 3(H_2O)
Formula weight	250.26
Temperature	193(2) K
Wavelength, radiation type	0.71073Å, MoKα
Diffractometer	STOE IPDS 2T
Crystal system	Monoclinic
Space group name, number	P 21/c, (14)
Unit cell dimensions	a = 14.3213(11) Å
	b = 6.9452(4) Å
	c = 12.6860(8) Å
Volume	1241.61(14) $Å^3$
Number of reflections	2671
and range used for lattice parameters	2.89° <=θ<= 27.85°
Z	4
Density (calculated)	1.339 Mg/m^3
Absorption coefficient	0.100 mm^{-1}
Absorption correction	None
F(000)	528
Crystal size, colour and form	0.060 x 0.100 x 0.450 mm^3, colourless plate
Theta range for data collection	2.891 to 28.297°.
Index ranges	-19<=h<=19, -9<=k<=8, -16<=l<=16
Number of reflections:	
collected	6513
independent	3058 [R(int) = 0.0451]
observed [I>2sigma(I)]	1545
Completeness to theta = 25.2°	99.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3058 / 6 / 205
Goodness-of-fit on F^2	0.953
Final R indices [I>2sigma(I)]	R1 = 0.0561, wR2 = 0.1277
R indices (all data)	R1 = 0.1258, wR2 = 0.1506
Largest diff. peak and hole	0.242 and -0.222 $eÅ^{-3}$

Table S2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
C1	0.46309(15)	0.6459(3)	0.17906(15)	0.0297(5)
N2	0.46650(14)	0.6781(3)	0.07740(13)	0.0382(5)
N3	0.37683(15)	0.6800(3)	0.01977(14)	0.0444(6)
C4	0.31782(18)	0.6504(4)	0.08750(17)	0.0382(6)
C5	0.21792(19)	0.6398(4)	0.0699(2)	0.0499(7)
C6	0.1745(2)	0.6069(5)	0.1548(3)	0.0570(8)
C7	0.2292(2)	0.5820(4)	0.2587(2)	0.0533(7)
C8	0.32435(19)	0.5910(4)	0.2765(2)	0.0403(6)
N9	0.36930(13)	0.6274(3)	0.19053(13)	0.0314(5)
C10	0.54768(15)	0.6371(3)	0.26141(16)	0.0290(5)
C11	0.55050(17)	0.6869(3)	0.36868(17)	0.0332(5)
C12	0.63698(18)	0.6827(4)	0.43786(18)	0.0378(6)
N13	0.71952(14)	0.6370(3)	0.40921(15)	0.0412(5)
C14	0.71635(19)	0.5883(4)	0.3059(2)	0.0395(6)
C15	0.63390(17)	0.5844(3)	0.23116(19)	0.0352(6)
O1W	0.89786(13)	0.6710(3)	0.53289(13)	0.0449(5)
O2W	0.92187(15)	0.9708(3)	0.68122(15)	0.0517(5)
O3W	0.98500(13)	0.3311(3)	0.62154(13)	0.0472(5)

Table S3. Anisotropic displacement parameters ($Å^2$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}
C1	0.0339(12)	0.0266(12)	0.0312(10)	-0.0016(9)
N2	0.0440(12)	0.0429(13)	0.0290(9)	0.0006(8)
N3	0.0525(14)	0.0487(14)	0.0315(10)	-0.0014(9)
C4	0.0437(15)	0.0359(14)	0.0338(11)	-0.0055(10)
C5	0.0384(16)	0.0494(18)	0.0583(16)	-0.0093(13)
C6	0.0343(16)	0.056(2)	0.079(2)	-0.0107(15)
C7	0.0458(17)	0.0550(19)	0.0636(17)	-0.0082(14)
C8	0.0429(16)	0.0417(15)	0.0399(13)	-0.0026(11)
N9	0.0348(11)	0.0295(11)	0.0309(9)	-0.0022(8)
C10	0.0332(13)	0.0244(12)	0.0307(10)	0.0010(9)
C11	0.0340(14)	0.0337(14)	0.0335(11)	-0.0004(9)
C12	0.0441(15)	0.0353(14)	0.0341(11)	-0.0019(10)
N13	0.0401(13)	0.0389(12)	0.0433(11)	-0.0019(9)
C14	0.0357(14)	0.0359(15)	0.0485(14)	0.0018(11)
C15	0.0410(15)	0.0317(13)	0.0352(12)	-0.0001(10)
O1W	0.0407(11)	0.0507(12)	0.0405(9)	0.0022(8)
O2W	0.0539(13)	0.0486(13)	0.0519(11)	-0.0032(9)
O3W	0.0487(12)	0.0549(13)	0.0372(9)	-0.0008(9)

Table S4. Hydrogen coordinates and isotropic displacement parameters (Å^2) for 1.

Atom	x	y	z	U(eq)
H5	0.181(2)	0.654(4)	-0.007(2)	0.060
H6	0.105(2)	0.603(4)	0.142(2)	0.068
H7	0.197(2)	0.537(4)	0.319(2)	0.064
H8	0.365(2)	0.580(4)	0.341(2)	0.048
H11	0.498(2)	0.731(4)	0.393(2)	0.040
H12	0.640(2)	0.717(4)	0.512(2)	0.045
H14	0.780(2)	0.558(4)	0.288(2)	0.047
H15	0.635(2)	0.552(3)	0.158(2)	0.042
H1W	0.924(2)	0.571(3)	0.566(2)	0.067
H2W	0.839(1)	0.651(4)	0.494(2)	0.067
H3W	0.951(2)	1.073(3)	0.669(2)	0.077
H4W	0.915(2)	0.876(4)	0.634(2)	0.077
H5W	1.019(2)	0.368(4)	0.676(2)	0.071
H6W	1.022(2)	0.314(5)	0.575(2)	0.071

Table S5. Bond lengths [Å] and angles [°] for 1.

Bond lengths [Å]		Bond angles [°]	
C1-N2	1.318(3)	N2-C1-N9	108.95(18)
C1-N9	1.383(3)	N2-C1-C10	122.61(19)
C1-C10	1.453(3)	N9-C1-C10	128.43(17)
N2-N3	1.360(3)	C1-N2-N3	109.36(19)
N3-C4	1.324(3)	C4-N3-N2	107.48(17)
C4-N9	1.391(3)	N3-C4-N9	109.6(2)
C4-C5	1.410(4)	N3-C4-C5	130.7(2)
C5-C6	1.355(4)	N9-C4-C5	119.7(2)
C5-H5	1.03(3)	C6-C5-C4	118.6(3)
C6-C7	1.419(4)	C6-C5-H5	122.1(15)
C6-H6	0.99(3)	C4-C5-H5	119.2(15)
C7-C8	1.342(4)	C5-C6-C7	120.2(3)
C7-H7	1.02(3)	C5-C6-H6	118.3(17)
C8-N9	1.385(3)	C7-C6-H6	121.5(17)
C8-H8	0.91(3)	C8-C7-C6	121.8(3)
C10-C11	1.398(3)	C8-C7-H7	118.3(17)
C10-C15	1.405(3)	C6-C7-H7	119.3(17)
C11-C12	1.385(3)	C7-C8-N9	118.4(2)
C11-H11	0.91(2)	C7-C8-H8	127.7(16)
C12-N13	1.336(3)	N9-C8-H8	113.8(16)
C12-H12	0.96(2)	C1-N9-C8	134.14(19)
N13-C14	1.346(3)	C1-N9-C4	104.64(17)
C14-C15	1.377(3)	C8-N9-C4	121.2(2)
C14-H14	1.01(3)	C11-C10-C15	117.1(2)
C15-H15	0.95(2)	C11-C10-C1	124.4(2)
O1W-H1W	0.862(17)	C15-C10-C1	118.37(18)
O1W-H2W	0.906(17)	C12-C11-C10	118.6(2)
O2W-H3W	0.856(18)	C12-C11-H11	119.7(14)
O2W-H4W	0.880(18)	C10-C11-H11	121.5(14)
O3W-H5W	0.812(18)	N13-C12-C11	124.6(2)
O3W-H6W	0.866(17)	N13-C12-H12	116.2(15)
		C11-C12-H12	119.2(15)
		C12-N13-C14	116.5(2)
		N13-C14-C15	123.5(2)
		N13-C14-H14	113.8(14)
		C15-C14-H14	122.7(14)

C14-C15-C10	119.6(2)
C14-C15-H15	121.0(15)
C10-C15-H15	119.3(15)
H1W-O1W-H2W	115(3)
H3W-O2W-H4W	120(3)
H5W-O3W-H6W	106(3)

Table S6. Torsion angles [°] for 1.

N9-C1-N2-N3	-0.5(3)
C10-C1-N2-N3	-179.5(2)
C1-N2-N3-C4	0.6(3)
N2-N3-C4-N9	-0.4(3)
N2-N3-C4-C5	179.7(3)
N3-C4-C5-C6	179.8(3)
N9-C4-C5-C6	0.0(4)
C4-C5-C6-C7	-0.7(4)
C5-C6-C7-C8	0.4(5)
C6-C7-C8-N9	0.6(4)
N2-C1-N9-C8	179.0(2)
C10-C1-N9-C8	-2.1(4)
N2-C1-N9-C4	0.2(2)
C10-C1-N9-C4	179.1(2)
C7-C8-N9-C1	-179.9(3)
C7-C8-N9-C4	-1.3(4)
N3-C4-N9-C1	0.1(3)
C5-C4-N9-C1	-180.0(2)
N3-C4-N9-C8	-178.9(2)
C5-C4-N9-C8	1.0(3)
N2-C1-C10-C11	150.7(2)
N9-C1-C10-C11	-28.0(4)
N2-C1-C10-C15	-25.9(3)
N9-C1-C10-C15	155.3(2)
C15-C10-C11-C12	0.4(3)
C1-C10-C11-C12	-176.3(2)
C10-C11-C12-N13	1.1(4)
C11-C12-N13-C14	-1.4(4)
C12-N13-C14-C15	0.1(4)
N13-C14-C15-C10	1.4(4)
C11-C10-C15-C14	-1.6(3)
C1-C10-C15-C14	175.3(2)

Table S7. Hydrogen bonds for 1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O1W-H1W...O3W	0.862(17)	1.954(18)	2.810(3)	172(3)
O1W-H2W...N13	0.906(17)	1.857(18)	2.759(3)	174(3)
O2W-H3W...O3W#1	0.856(18)	1.98(2)	2.810(3)	164(3)
O2W-H4W...O1W	0.880(18)	1.906(18)	2.786(3)	179(3)
O3W-H5W...O2W#2	0.812(18)	1.991(19)	2.791(3)	169(3)
O3W-H6W...O1W#3	0.866(17)	1.942(18)	2.797(3)	169(3)

Symmetry transformations used to generate equivalent atoms:

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

Table S8. Crystal data and structure refinement for 2.

CCDC code	204925
Empirical formula	$C_{11}H_{13}BrN_4O_3$
moiety formula	$C_{11}H_7BrN_4$, 3(H_2O)
Formula weight	329.16
Temperature	193(2) K
Wavelength, radiation type	0.71073Å, MoKα
Diffractometer	STOE IPDS 2T
Crystal system	Monoclinic
Space group name, number	P 21/c, (14)
Unit cell dimensions	a = 15.1413(12) Å
	b = 6.9179(4) Å
	c = 13.0938(8) Å
Volume	1324.16(16) $Å^3$
Number of reflections	10813
and range used for lattice parameters	2.79° <=θ<= 28.30°
Z	4
Density (calculated)	1.651 Mg/m^3
Absorption coefficient	3.115 mm^{-1}
Absorption correction	Integration
Max. and min. transmission	0.7525 and 0.3237
F(000)	664
Crystal size, colour and form	0.100 x 0.320 x 0.340 mm^3, colourless plate
Theta range for data collection	2.787 to 28.270°.
Index ranges	-20<=h<=16, -9<=k<=9, -17<=l<=17
Number of reflections:	
collected	6912
independent	3252 [R(int) = 0.0167]
observed [I>2sigma(I)]	2727
Completeness to theta = 25.2°	99.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3252 / 15 / 221
Goodness-of-fit on F^2	1.126
Final R indices [I>2sigma(I)]	R1 = 0.0337, wR2 = 0.0679
R indices (all data)	R1 = 0.0463, wR2 = 0.0740
Largest diff. peak and hole	0.414 and -0.472 $eÅ^{-3}$

Table S9. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for 2. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
Br1	0.19016(2)	0.50988(4)	0.29226(2)	0.03244(8)
C1	0.48154(16)	0.3302(3)	0.15510(17)	0.0220(4)
N2	0.48914(14)	0.2848(3)	0.05977(15)	0.0266(4)
N3	0.40356(15)	0.2781(3)	-0.00856(15)	0.0283(4)
C4	0.34436(17)	0.3216(3)	0.04701(17)	0.0240(5)
C5	0.24865(18)	0.3430(4)	0.0151(2)	0.0300(5)
C6	0.20330(18)	0.3960(4)	0.0872(2)	0.0301(5)
C7	0.25373(17)	0.4291(3)	0.19352(19)	0.0245(5)
C8	0.34516(16)	0.4079(3)	0.22636(18)	0.0220(4)
N9	0.39053(13)	0.3536(3)	0.15181(14)	0.0206(4)
C10	0.56116(15)	0.3556(3)	0.24515(17)	0.0208(4)
C11	0.56147(16)	0.3177(3)	0.35009(18)	0.0225(4)
C12	0.64329(17)	0.3331(3)	0.42755(19)	0.0258(5)
N13	0.72308(14)	0.3813(3)	0.40792(16)	0.0266(4)
C14	0.72165(18)	0.4220(3)	0.3069(2)	0.0272(5)
C15	0.64347(17)	0.4118(3)	0.22508(19)	0.0245(5)
O1W	0.90122(13)	0.3325(3)	0.53186(14)	0.0323(4)
O2W	0.92288(16)	0.0243(3)	0.67136(17)	0.0449(5)
O3W	1.00321(14)	0.3335(3)	0.38121(15)	0.0359(4)

Table S10. Anisotropic displacement parameters (Å^2) for 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}
Br1	0.03013(13)	0.03722(14)	0.03526(13)	0.00485(11)
C1	0.0267(12)	0.0214(10)	0.0208(10)	0.0023(8)
N2	0.0331(11)	0.0283(10)	0.0211(9)	-0.0003(8)
N3	0.0348(11)	0.0307(10)	0.0201(9)	-0.0023(8)
C4	0.0318(12)	0.0224(10)	0.0174(10)	-0.0015(8)
C5	0.0343(14)	0.0280(12)	0.0240(12)	-0.0027(10)
C6	0.0266(13)	0.0277(12)	0.0336(13)	0.0011(10)
C7	0.0283(12)	0.0204(10)	0.0274(11)	0.0029(9)
C8	0.0265(11)	0.0216(10)	0.0188(10)	0.0019(8)
N9	0.0249(10)	0.0190(8)	0.0187(8)	0.0006(7)
C10	0.0253(11)	0.0170(9)	0.0218(10)	0.0008(8)
C11	0.0245(11)	0.0218(10)	0.0239(11)	0.0013(8)
C12	0.0297(12)	0.0257(11)	0.0228(11)	0.0012(9)
N13	0.0257(10)	0.0265(10)	0.0275(10)	-0.0019(8)
C14	0.0267(12)	0.0240(11)	0.0340(13)	-0.0010(10)
C15	0.0297(12)	0.0224(10)	0.0245(11)	0.0029(9)
O1W	0.0256(9)	0.0385(10)	0.0318(10)	-0.0007(8)
O2W	0.0490(13)	0.0393(11)	0.0376(11)	-0.0034(9)
O3W	0.0397(11)	0.0389(11)	0.0317(10)	-0.0067(8)

Table S11. Hydrogen coordinates and isotropic displacement parameters (Å^2) for 2.

Atom	x	y	z	U(eq)
H5	0.222(2)	0.327(4)	-0.053(2)	0.032(7)
H6	0.140(2)	0.411(5)	0.070(2)	0.041(8)
H8	0.377(2)	0.428(4)	0.293(2)	0.023(7)
H11	0.507(2)	0.278(4)	0.367(2)	0.023(6)
H12	0.646(2)	0.305(4)	0.495(2)	0.031(7)
H14	0.777(2)	0.457(4)	0.294(2)	0.026(7)
H15	0.644(2)	0.445(4)	0.158(2)	0.033(8)
H1W	0.847(1)	0.347(5)	0.500(2)	0.053(7)
H2W	0.911(2)	0.239(4)	0.571(2)	0.053(7)
H3W	0.949(3)	0.062(6)	0.731(2)	0.076(10)
H4W	0.949(3)	-0.073(4)	0.660(3)	0.076(10)
H5W	0.970(2)	0.321(5)	0.421(2)	0.055(7)
H6W	1.039(2)	0.421(4)	0.407(3)	0.055(7)

Table S12. Bond lengths [Å] and angles [°] for 2.

Bond lengths [Å]		Bond angles [°]	
Br1-C7	1.886(2)	N2-C1-N9	109.3(2)
C1-N2	1.321(3)	N2-C1-C10	122.3(2)
C1-N9	1.377(3)	N9-C1-C10	128.30(19)
C1-C10	1.461(3)	C1-N2-N3	108.95(19)
N2-N3	1.370(3)	C4-N3-N2	107.04(18)
N3-C4	1.328(3)	N3-C4-N9	109.9(2)
C4-N9	1.386(3)	N3-C4-C5	130.6(2)
C4-C5	1.408(4)	N9-C4-C5	119.5(2)
C5-C6	1.354(4)	C6-C5-C4	119.4(2)
C5-H5	0.88(3)	C6-C5-H5	123.5(19)
C6-C7	1.422(4)	C4-C5-H5	116.9(19)
C6-H6	0.93(3)	C5-C6-C7	119.1(2)
C7-C8	1.346(3)	C5-C6-H6	122.7(19)
C8-N9	1.384(3)	C7-C6-H6	118.2(19)
C8-H8	0.89(3)	C8-C7-C6	122.7(2)
C10-C15	1.394(3)	C8-C7-Br1	118.63(18)
C10-C11	1.398(3)	C6-C7-Br1	118.65(18)
C11-C12	1.386(3)	C7-C8-N9	117.5(2)
C11-H11	0.95(3)	C7-C8-H8	123.0(18)
C12-N13	1.341(3)	N9-C8-H8	119.5(18)
C12-H12	0.89(3)	C1-N9-C8	133.4(2)
N13-C14	1.347(3)	C1-N9-C4	104.76(18)
C14-C15	1.376(4)	C8-N9-C4	121.8(2)
C14-H14	0.93(3)	C15-C10-C11	117.6(2)
C15-H15	0.91(3)	C15-C10-C1	118.1(2)
O1W-H1W	0.826(19)	C11-C10-C1	124.2(2)
O1W-H2W	0.814(19)	C12-C11-C10	118.6(2)
O2W-H3W	0.82(2)	C12-C11-H11	121.0(16)
O2W-H4W	0.81(2)	C10-C11-H11	120.4(16)
O3W-H5W	0.817(19)	N13-C12-C11	123.9(2)
O3W-H6W	0.825(19)	N13-C12-H12	115.6(19)
		C11-C12-H12	120.5(19)
		C12-N13-C14	117.1(2)
		N13-C14-C15	123.0(2)
		N13-C14-H14	116.7(17)

C15-C14-H14	120.3(17)
C14-C15-C10	119.8(2)
C14-C15-H15	120.8(19)
C10-C15-H15	119.3(19)
H1W-O1W-H2W	114(4)
H3W-O2W-H4W	107(4)
H5W-O3W-H6W	105(3)

Table S13. Torsion angles [°] for 2.

N9-C1-N2-N3	0.3(3)
C10-C1-N2-N3	-177.8(2)
C1-N2-N3-C4	0.4(3)
N2-N3-C4-N9	-1.0(3)
N2-N3-C4-C5	177.1(2)
N3-C4-C5-C6	-177.4(3)
N9-C4-C5-C6	0.5(4)
C4-C5-C6-C7	0.1(4)
C5-C6-C7-C8	-0.8(4)
C5-C6-C7-Br1	178.25(19)
C6-C7-C8-N9	0.7(4)
Br1-C7-C8-N9	-178.29(15)
N2-C1-N9-C8	-176.9(2)
C10-C1-N9-C8	1.0(4)
N2-C1-N9-C4	-0.9(2)
C10-C1-N9-C4	177.0(2)
C7-C8-N9-C1	175.5(2)
C7-C8-N9-C4	-0.1(3)
N3-C4-N9-C1	1.2(2)
C5-C4-N9-C1	-177.2(2)
N3-C4-N9-C8	177.8(2)
C5-C4-N9-C8	-0.6(3)
N2-C1-C10-C15	26.6(3)
N9-C1-C10-C15	-151.0(2)
N2-C1-C10-C11	-150.0(2)
N9-C1-C10-C11	32.4(4)
C15-C10-C11-C12	-1.6(3)
C1-C10-C11-C12	175.0(2)
C10-C11-C12-N13	-0.5(4)
C11-C12-N13-C14	2.0(4)
C12-N13-C14-C15	-1.5(4)
N13-C14-C15-C10	-0.5(4)
C11-C10-C15-C14	2.1(3)
C1-C10-C15-C14	-174.7(2)

Table S14. Hydrogen bonds for 2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O1W-H1W...N13	0.826(19)	1.96(2)	2.783(3)	173(3)
O1W-H2W...O2W	0.814(19)	1.96(2)	2.771(3)	174(4)
O2W-H3W...O3W#1	0.82(2)	2.06(2)	2.873(3)	175(4)
O2W-H4W...O3W#2	0.81(2)	2.07(2)	2.873(3)	171(4)
O3W-H5W...O1W	0.817(19)	2.00(2)	2.804(3)	170(4)
O3W-H6W...O1W#3	0.825(19)	2.00(2)	2.805(3)	167(4)

Supplementary Information

Symmetry transformations used to generate equivalent atoms:

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