Phenanthroline Unit as a Building Block for Carbohydrate Receptors

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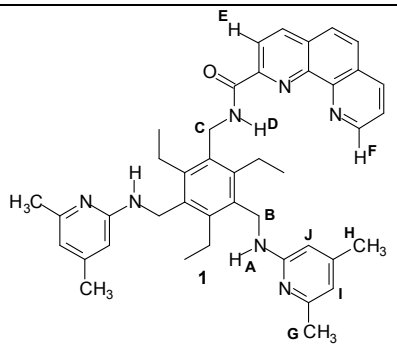


1. Further examples of ^{1}H NMR titrations of **1** with monosaccharides **2a**, **3a** and **4a**

The binding studies were carried out in $CDCl_3$, water-containing $CDCl_3$, DMSO-d_6/$CDCl_3$ and CD_3OD/$CDCl_3$ mixtures (0.1:9.9, 0.5:9.5, and 1:9 v/v) at 25°C. The titration data were analyzed by non-linear regression analysis, using the program HOSTEST 5.6 (Wilcox, C. S.; Glagovich, N. M. Program HOSTEST 5.6; University of Pittsburgh: Pittsburgh, PA, 1994). The stoichiometry of receptor-sugar complexes was determined by mole ratio method and by the curve-fitting analysis of the titration data. For each system at least 3 titrations were carried out; for each titration 16-20 samples were prepared. Dilution experiments show that receptor **1** does not self-aggregate in the used concentration range.

1.1 ^{1}H NMR titrations of **1** with β-glucopyranoside **2a** ($CDCl_3$).

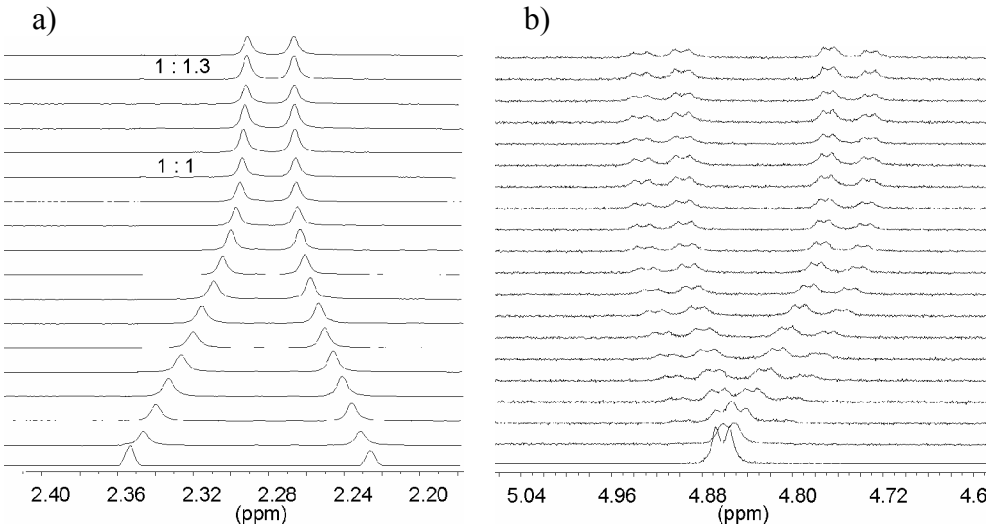


Figure S1. (a,b) Partial ^{1}H NMR spectra (400 MHz, $CDCl_3$) of receptor **1** (1.00 mM) after addition of (from bottom to top) 0.00–1.50 equiv of β-glucopyranoside **2a**. Shown are chemical shifts of the $CH_3^{G,H}$, and CH_2^{C} signals of **1** (for labeling, see Figure 1).

1.2 ^{1}H NMR titrations of **1** with α-glucopyranoside **3a** ($CDCl_3$, water-containing $CDCl_3$ or DMSO-d_6/$CDCl_3$).

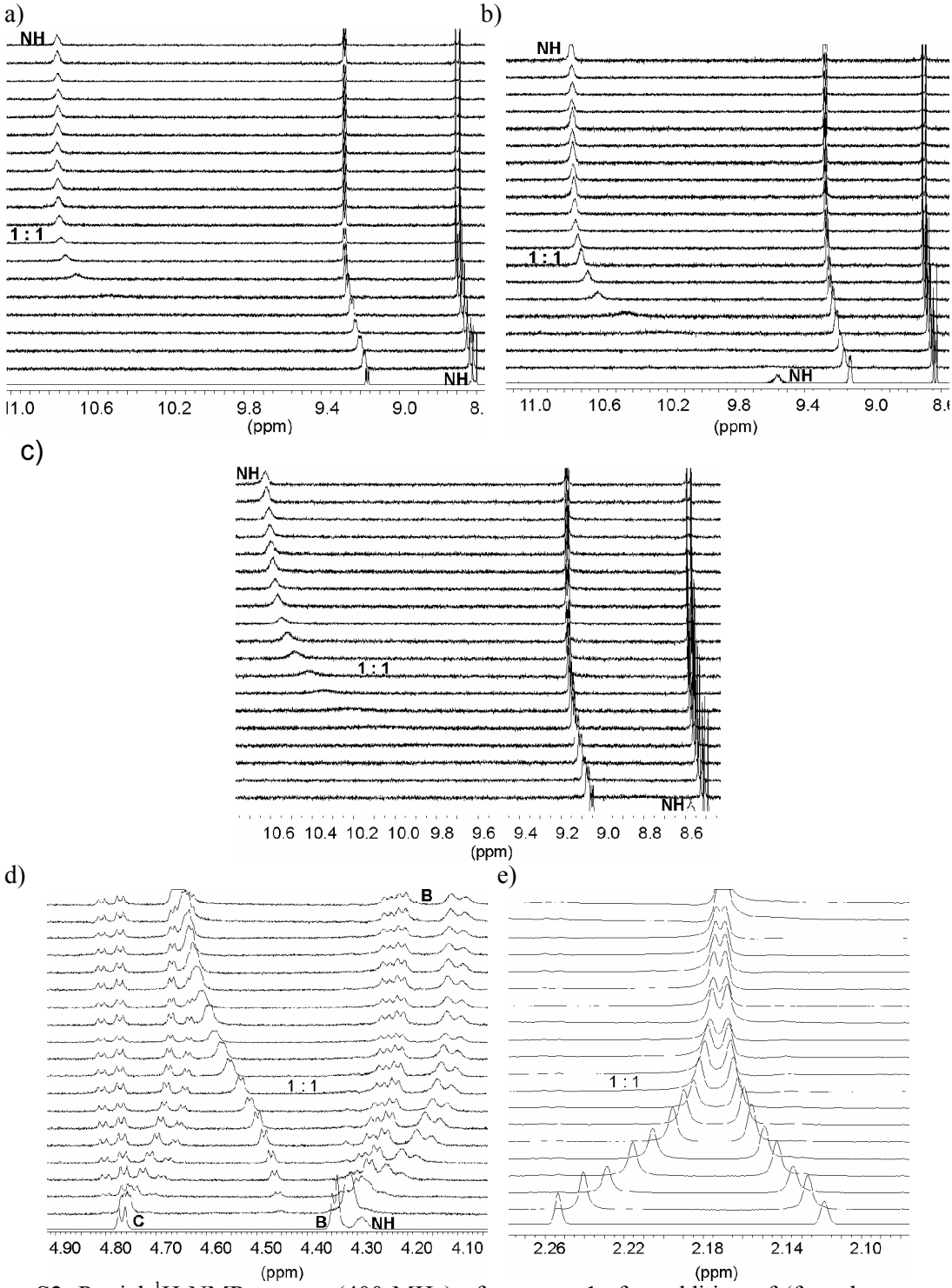


Figure S2. Partial ^{1}H NMR spectra (400 MHz) of receptor **1** after addition of (from bottom to top) 0.00 – 2.60 equiv of α-glucopyranoside **3a**: (a) $CDCl_3$, (b) water-containing $CDCl_3$ (0.04 % H_2O), (c-e) DMSO-d_6/$CDCl_3$, 0.5:9.5 v/v ([**1**] = 1.01 mM). Shown are chemical shifts of the NH^{D}, and $CH^{F,E}$, $CH_2{}^{C,B}$, and $CH_3{}^{G,H}$ signals of **1**.

1.3 ^{1}H NMR titrations of receptor **1** with β-glucopyranoside **2a** and β-galactopyranoside **4a** (DMSO-d_6/$CDCl_3$ or $CDCl_3$).

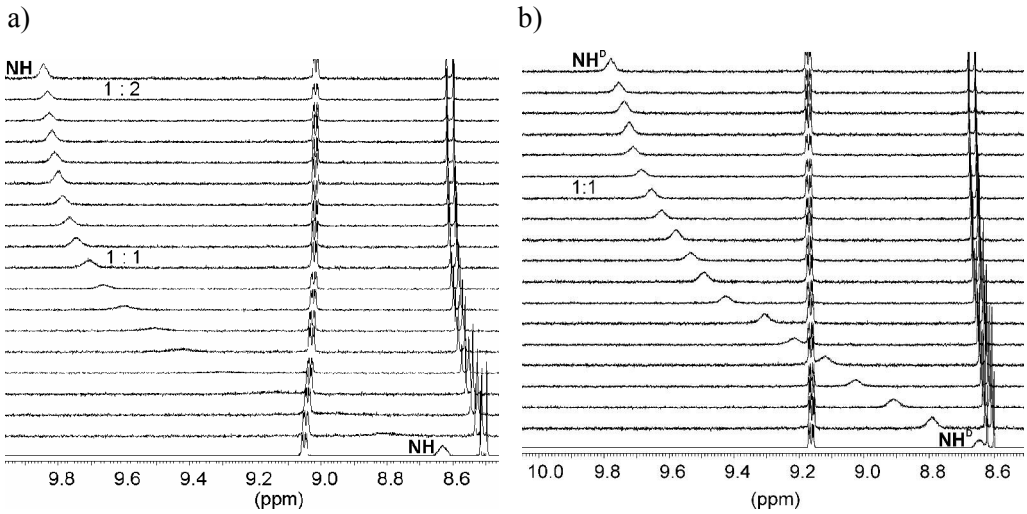
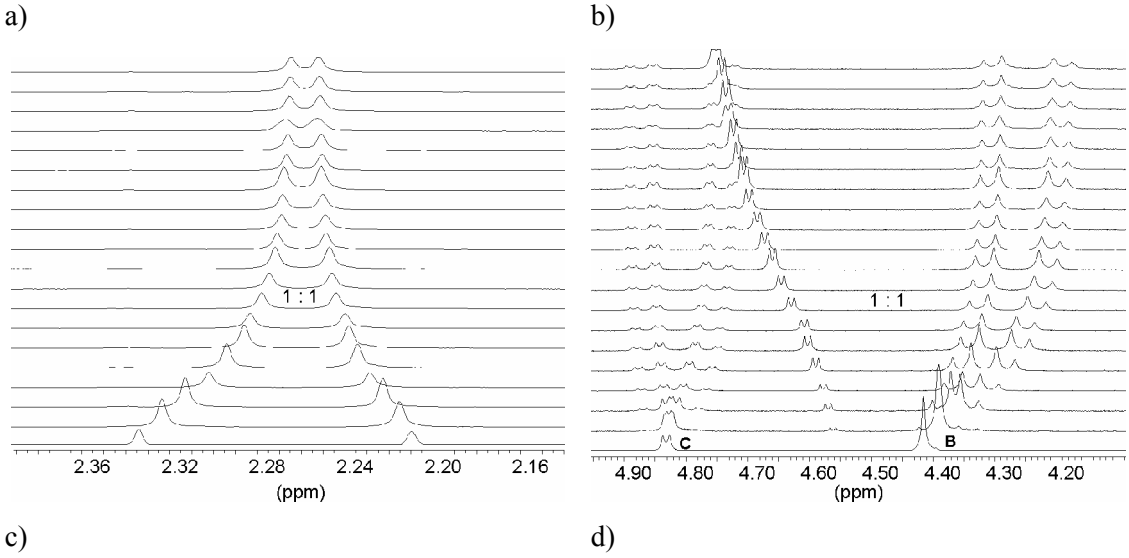


Figure S3. (a) Partial ^{1}H NMR spectra (400 MHz; DMSO-d_6/$CDCl_3$, 0.5:9.5, v/v) of receptor **1** after addition of (from bottom to top) 0.00–2.35 equiv of β-glucopyranoside **2a** ([**1**] = 1.00 mM). (b) ^{1}H NMR spectra (400 MHz; $CDCl_3$) of receptor **1** after addition of 0.00–1.80 equiv of β-galactopyranoside **4a** ([**1**] = 0.90 mM). Shown are chemical shifts of the NH^D, and $CH^{F,E}$ signals (for labeling, see formula **1**).

1.4 ^{1}H NMR titrations of receptor **1** with α-glucopyranoside **3a** (1% and 5% CD_3OD in $CDCl_3$).



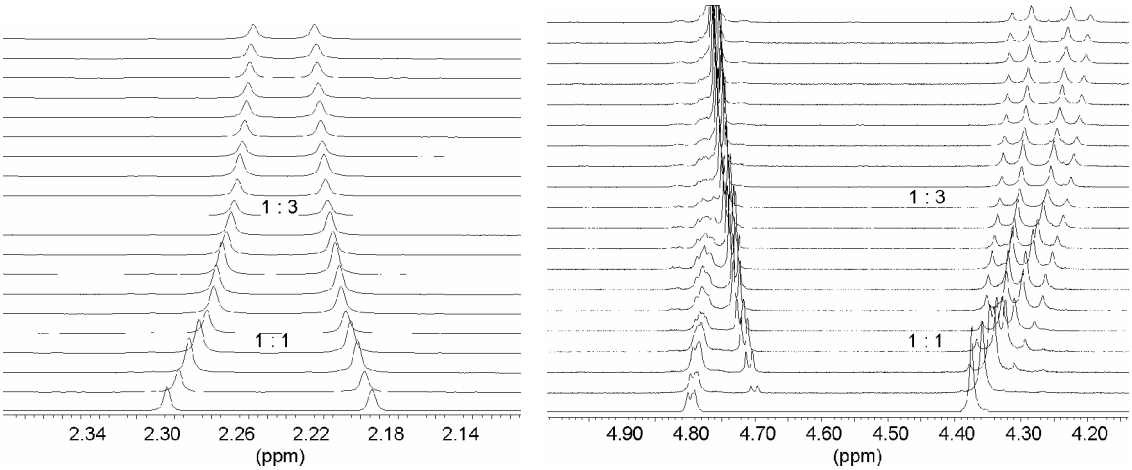


Figure S4. (a, b) Partial ^{1}H NMR spectra (400 MHz; $CD_3OD/CDCl_3$, 0.1:9.9, v/v) of receptor **1** after addition of (from bottom to top) 0.00–2.84 equiv of α-glucopyranoside **3a** ([**1**] = 1.03 mM). (b, c) ^{1}H NMR spectra (400 MHz; $CD_3OD/CDCl_3$, 0.5:9.5, v/v) of receptor **1** after addition of 0.00–6.50 equiv of α-glucopyranoside **3a** ([**1**] = 1.05 mM). Shown are chemical shifts of the $CH_3^{G,H}$ and $CH_2^{B,C}$ signals of **1**.

2 ^{1}H NMR titrations of β-glucopyranoside **2a** and α-glucopyranoside **3a** with receptor **1** (inverse titrations in $CDCl_3$)

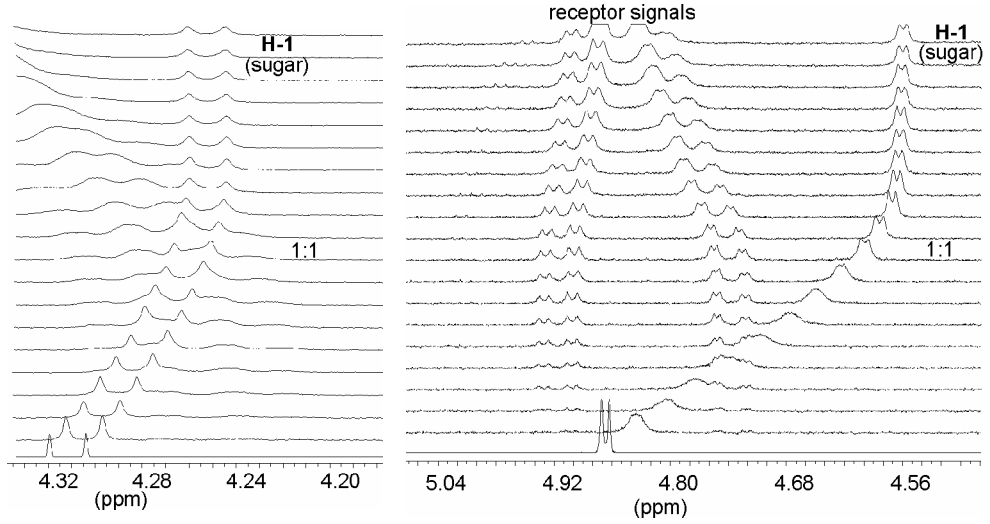


Figure S5. Partial ^{1}H NMR spectra (500 MHz; $CDCl_3$) of β-glucopyranoside **2a** (left) and α-glucopyranoside **3a** (right) after addition of 0.00-3.30 equiv of **1** (inverse titrations; [**2a**] = 0.69 mM, [**3a**] = 0.68 mM).

3. Representative mole ratio plots.

a) b)

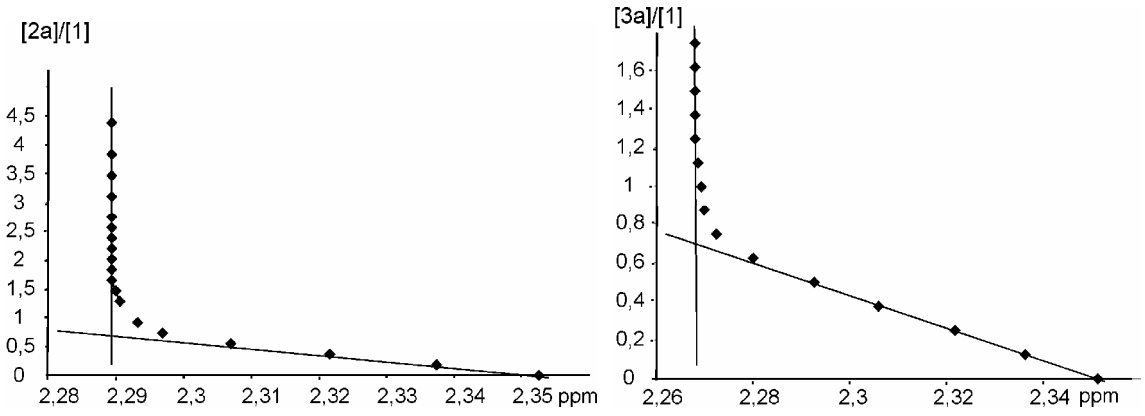


Figure S6. Mole ratio plots: (a) titration of **1** with β-glucopyranoside **2a**, (b) titration of receptor **1** with α-glucopyranoside **3a** (analysis of the shifts of the CH_3 protons of **1**).

4. Extraction experiments

Extraction of sugars from the solid state into a 1.1 mM $CDCl_3$ solution of receptor **1** (control experiments were performed in the absence of **1**).

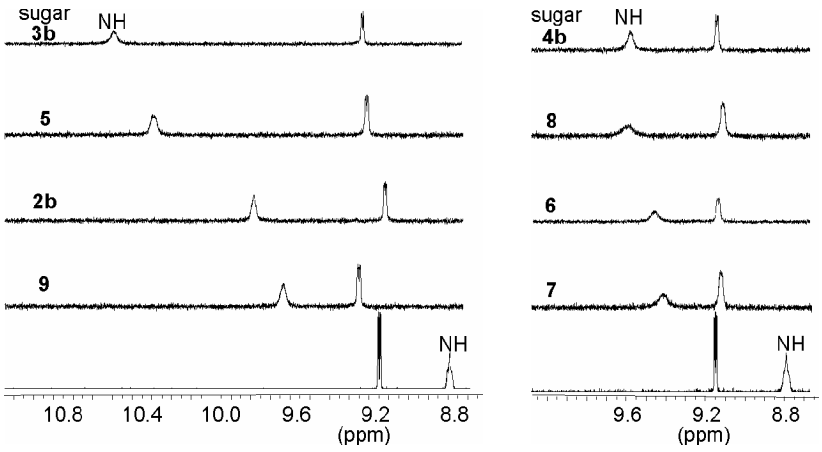


Figure S7. Partial ^{1}H NMR spectra (400 MHz) of receptor **1** before (bottom) and after the extraction of solid methyl β-D-glucopyranoside (**2b**), methyl α-D-glucopyranoside (**3b**), methyl β-D-galactopyranoside (**4b**), methyl α-D-galactopyranoside (**5**), methyl α-D-mannopyranoside (**6**), *N*-acetyl-D-glucosamine (**7**), *N*-acetyl-D-galactosamine (**8**), and L-fucose (**9**) by a $CDCl_3$-solution of receptor **1** (1.10 mM). Shown are chemical shifts of the NH^D and CH^F signals of **1**.

5. Examples of hydrogen-bonding motifs indicated by molecular modeling studies

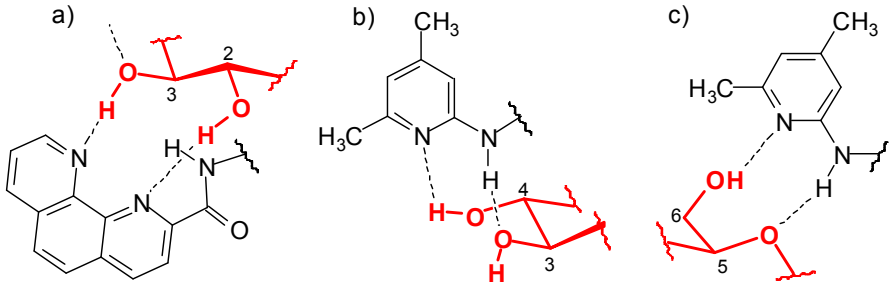
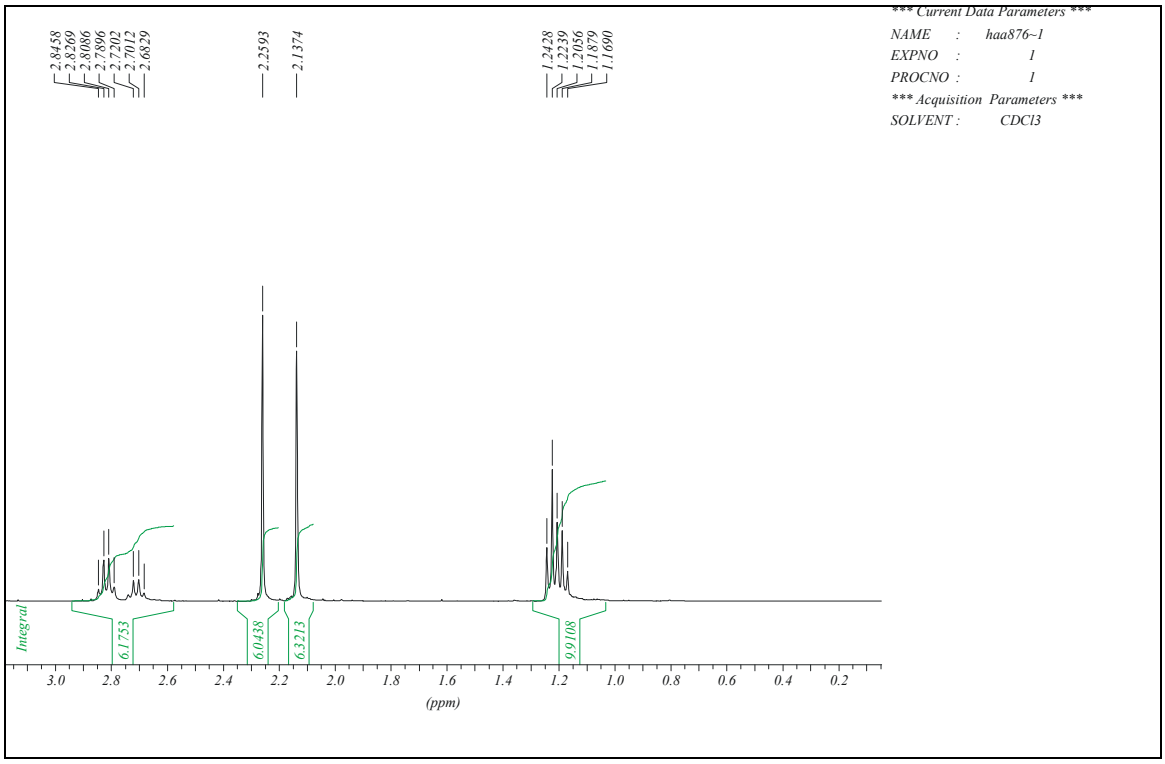


Figure S8. Examples of hydrogen-bonding motifs indicated by molecular modeling studies in the 1:1 complex between receptor **1** and β-glucopyranoside **2a** (MacroModel V.8.5, OPLS-AA force field, MCMM, 50000 steps).

6. ^{1}H and ^{13}C NMR Spectra of compound **1**.



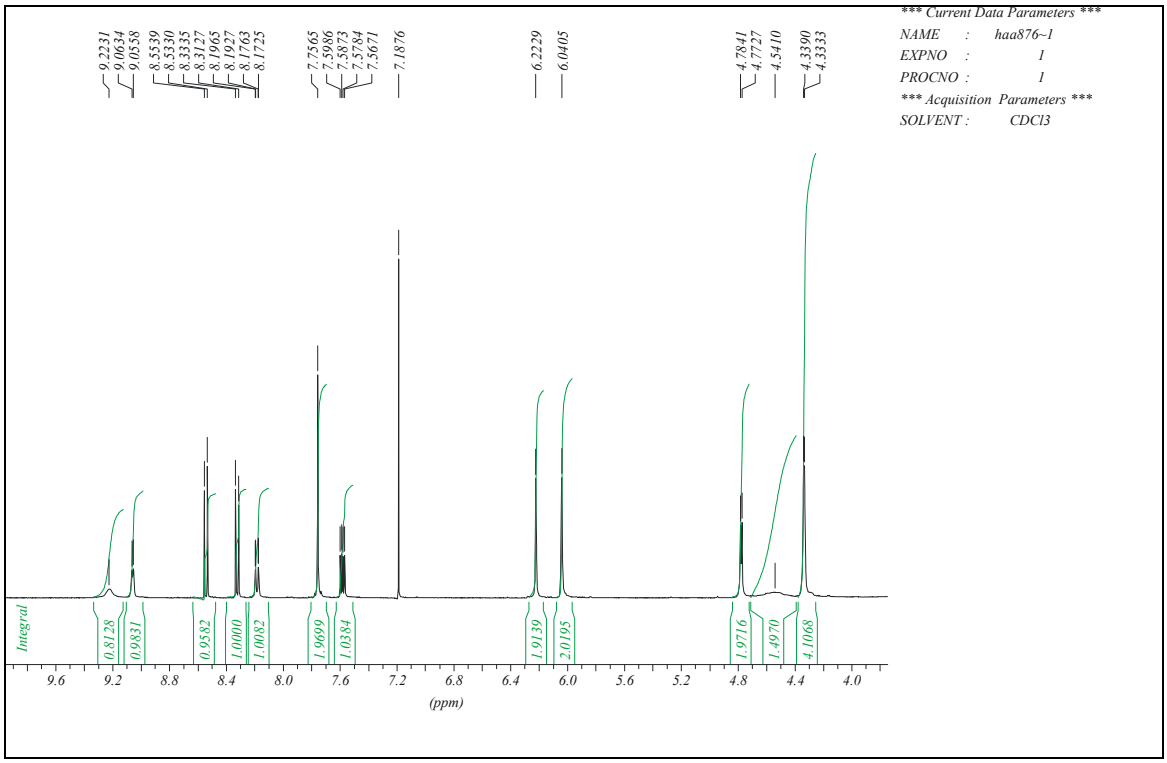


Figure S9. ^{1}H NMR spectrum of **1** (400 MHz, $CDCl_3$).

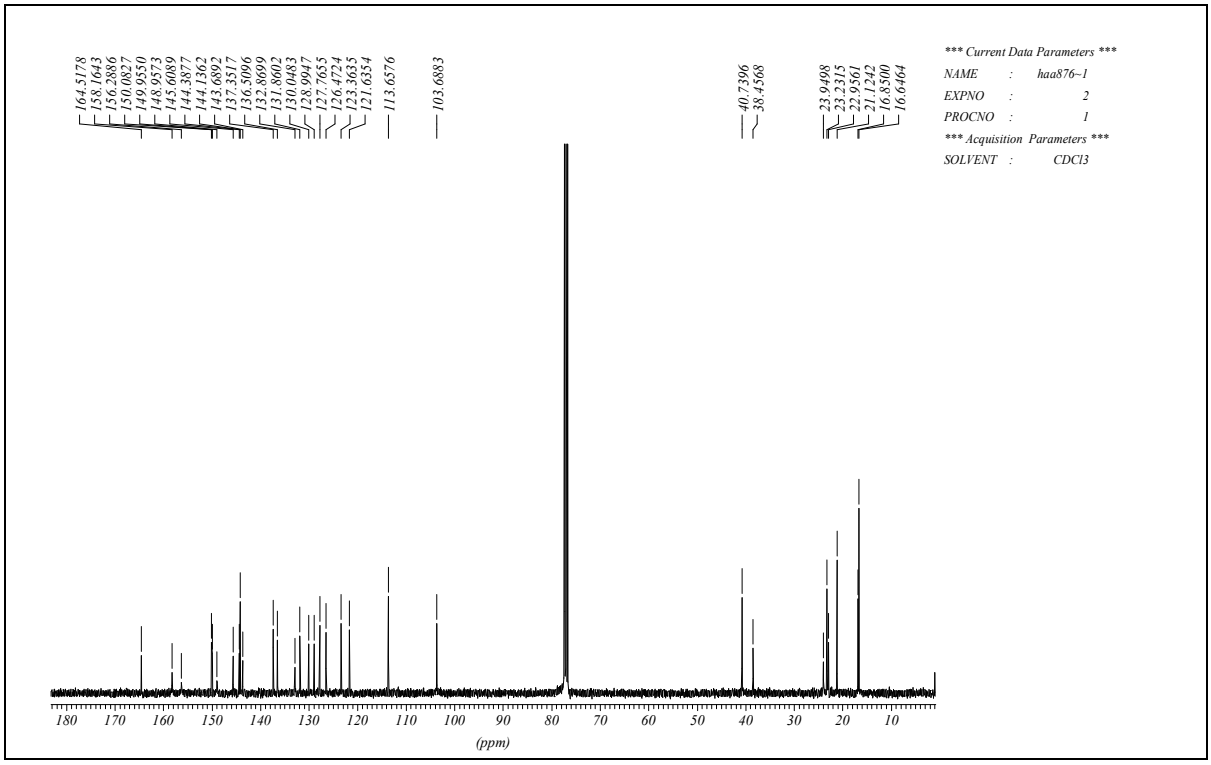


Figure S10. ^{13}C NMR spectrum of **1** (400 MHz, $CDCl_3$).

7. Crystal data and structure refinement for compound **1**.

Table 1. Crystal data and structure refinement.

Identification code	hope	
Empirical formula	$C_{44}H_{58}N_7O_{4.5}$	
Formula weight	756.97	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P(-1)	
Unit cell dimensions	a = 8.5389(9) Å	α= 78.454(4)°
	b = 11.0794(12) Å	β= 81.613(5)°
	c = 22.400(3) Å	γ = 86.883(4)°
Volume	2053.4(4) $Å^3$	
Z	2	
Density (calculated)	1.224 Mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	814	
Crystal size	0.43 x 0.38 x 0.20 mm^3	
Theta range for data collection	1.87 to 30.54°	
Index ranges	-12<=h<=12, -15<=k<=15, -31<=l<=32	
Reflections collected	29535	
Independent reflections	12337 [R(int) = 0.0494]	
Completeness to theta = 30.00°	98.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12337 / 24 / 541	
Goodness-of-fit on F^2	1.004	
Final R indices [I>2sigma(I)]	R1 = 0.0504, wR2 = 0.1175	
R indices (all data)	R1 = 0.0960, wR2 = 0.1356	
Largest diff. peak and hole	0.374 and -0.325 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1)	10339.0(12)	2713.5(9)	3537.9(5)	32.6(2)
N(1)	2223.9(13)	7350.8(10)	3006.7(5)	22.7(2)
C(2)	1076.3(17)	8015.6(13)	3293.5(6)	25.9(3)
C(3)	1100(2)	9388.7(14)	3070.4(8)	37.7(4)
C(4)	-57.3(17)	7474.4(14)	3759.0(7)	30.7(3)
C(5)	-52.9(17)	6187.8(14)	3946.6(7)	29.6(3)
C(6)	-1331(2)	5580.3(17)	4432.7(8)	44.0(4)

C(7)	1094.1(17)	5510.0(13)	3657.9(6)	26.0(3)
C(8)	2215.3(16)	6119.7(12)	3185.2(6)	22.5(3)
N(9)	3370.3(15)	5451.0(11)	2894.0(6)	28.9(3)
C(10)	4452.4(17)	6013.5(12)	2352.2(6)	26.5(3)
C(11)	5403.4(16)	4991.7(11)	2099.7(6)	22.2(3)
C(12)	4840.4(16)	4468.7(12)	1652.7(6)	21.3(3)
C(13)	3340.2(18)	4984.9(14)	1392.0(7)	31.5(3)
C(14)	3688(2)	6041.9(18)	837.3(8)	54.9(5)
C(15)	5669.9(15)	3467.4(11)	1450.8(6)	19.9(3)
C(16)	5059.2(17)	2896.2(12)	972.3(6)	24.2(3)
N(17)	3970.9(16)	1925.4(12)	1275.5(6)	31.5(3)
C(18)	3332.3(16)	1167.6(12)	969.1(6)	24.2(3)
C(19)	3574.2(17)	1338.9(13)	325.7(6)	25.8(3)
C(20)	2896.3(17)	534.6(13)	42.6(6)	26.6(3)
C(21)	3110(2)	698.4(15)	-646.4(7)	35.6(4)
C(22)	2005.2(18)	-419.0(13)	416.1(7)	30.2(3)
C(23)	1831.7(17)	-542.4(13)	1046.6(7)	28.6(3)
C(24)	866(2)	-1540.9(14)	1470.0(8)	39.0(4)
N(25)	2493.9(14)	234.3(11)	1327.6(5)	26.9(3)
C(26)	7002.6(16)	2942.7(11)	1713.3(6)	20.1(3)
C(27)	7824.7(17)	1809.4(12)	1516.7(6)	26.3(3)
C(28)	9143.1(19)	2133.7(14)	974.2(7)	34.8(4)
C(29)	7559.8(16)	3479.8(11)	2155.7(6)	20.9(3)
C(30)	8979.8(16)	2913.0(13)	2452.9(6)	25.4(3)
N(31)	8450.6(14)	2120.3(10)	3048.3(5)	24.3(3)
C(32)	9157.7(16)	2101.7(12)	3541.9(6)	23.8(3)
C(34)	8458.5(16)	1292.9(12)	4131.4(6)	23.6(3)
N(35)	7536.5(13)	393.8(10)	4087.9(5)	23.3(2)
C(36)	6977.4(16)	-386.8(12)	4614.8(6)	23.5(3)
C(37)	6019.7(16)	-1402.5(13)	4573.0(6)	24.5(3)
N(38)	5676.2(14)	-1487.5(11)	4010.4(5)	28.8(3)
C(39)	4824.1(18)	-2431.6(14)	3976.1(7)	33.7(3)
C(40)	4257.1(18)	-3333.4(14)	4484.2(8)	36.1(4)
C(41)	4594.0(18)	-3243.5(14)	5051.4(8)	34.2(4)
C(42)	5494.1(17)	-2262.0(13)	5112.5(7)	28.4(3)
C(43)	5874.7(18)	-2098.2(14)	5693.9(7)	33.2(3)
C(44)	6734.3(18)	-1139.1(15)	5734.0(7)	33.0(3)
C(45)	7318.0(16)	-261.2(13)	5196.4(6)	26.3(3)
C(46)	8256.3(17)	727.4(14)	5222.0(7)	29.3(3)

C(47)	8844.1(17)	1498.3(13)	4690.5(7)	27.7(3)
C(48)	6767.9(16)	4503.8(11)	2348.5(6)	21.5(3)
C(49)	7399.8(18)	5122.4(13)	2810.5(6)	28.8(3)
C(50)	8468(2)	6191.8(14)	2480.2(8)	40.0(4)
O(1W)	5637.9(14)	616.0(10)	2958.2(5)	36.1(3)
O(2W)	4576.8(13)	-913.2(10)	2230.2(5)	33.8(3)
O(3W)	3169.4(17)	2564.4(16)	2710.1(7)	73.0(5)
C(91)	-1871(5)	6005(4)	626(2)	47.2(10)
C(92)	-210(4)	5495(3)	509.9(16)	39.8(8)
O(93)	77(6)	5074(4)	15(2)	33.7(5)
C(94)	1448(4)	4487(3)	-182.1(15)	36.2(7)
C(95)	1417(5)	3905(4)	-735.6(18)	41.6(9)

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

O(1)-C(32)	1.2435(16)	C(23)-C(24)	1.501(2)
N(1)-C(8)	1.3425(17)	C(26)-C(29)	1.4024(18)
N(1)-C(2)	1.3575(18)	C(26)-C(27)	1.5161(19)
C(2)-C(4)	1.379(2)	C(27)-C(28)	1.531(2)
C(2)-C(3)	1.503(2)	C(29)-C(48)	1.3995(19)
C(4)-C(5)	1.403(2)	C(29)-C(30)	1.5144(18)
C(5)-C(7)	1.368(2)	C(30)-N(31)	1.4672(17)
C(5)-C(6)	1.507(2)	N(31)-C(32)	1.3310(17)
C(7)-C(8)	1.4079(19)	C(32)-C(34)	1.5026(19)
C(8)-N(9)	1.3687(18)	C(34)-N(35)	1.3297(17)
N(9)-C(10)	1.4654(18)	C(34)-C(47)	1.4041(19)
C(10)-C(11)	1.5112(19)	N(35)-C(36)	1.3567(17)
C(11)-C(48)	1.4003(19)	C(36)-C(45)	1.4102(19)
C(11)-C(12)	1.4043(18)	C(36)-C(37)	1.4521(19)
C(12)-C(15)	1.3996(18)	C(37)-N(38)	1.3569(17)
C(12)-C(13)	1.5212(19)	C(37)-C(42)	1.4130(19)
C(13)-C(14)	1.533(2)	N(38)-C(39)	1.3269(18)
C(15)-C(26)	1.4018(18)	C(39)-C(40)	1.402(2)
C(15)-C(16)	1.5140(17)	C(40)-C(41)	1.367(2)
C(16)-N(17)	1.4540(17)	C(41)-C(42)	1.405(2)
N(17)-C(18)	1.3651(17)	C(42)-C(43)	1.435(2)
C(18)-N(25)	1.3443(17)	C(43)-C(44)	1.348(2)
C(18)-C(19)	1.4013(19)	C(44)-C(45)	1.433(2)
C(19)-C(20)	1.3859(18)	C(45)-C(46)	1.407(2)

C(20)-C(22)	1.394(2)	C(46)-C(47)	1.365(2)
C(20)-C(21)	1.502(2)	C(48)-C(49)	1.5227(18)
C(22)-C(23)	1.378(2)	C(49)-C(50)	1.534(2)
C(23)-N(25)	1.3529(17)		
C(8)-N(1)-C(2)	117.54(12)	C(5)-C(7)-C(8)	119.29(13)
N(1)-C(2)-C(4)	122.53(13)	N(1)-C(8)-N(9)	117.43(12)
N(1)-C(2)-C(3)	115.99(13)	N(1)-C(8)-C(7)	122.76(13)
C(4)-C(2)-C(3)	121.48(13)	N(9)-C(8)-C(7)	119.80(12)
C(2)-C(4)-C(5)	119.66(14)	C(8)-N(9)-C(10)	122.36(11)
C(7)-C(5)-C(4)	118.22(13)	N(9)-C(10)-C(11)	108.06(11)
C(7)-C(5)-C(6)	121.51(14)	C(48)-C(11)-C(12)	120.33(12)
C(4)-C(5)-C(6)	120.21(15)	C(48)-C(11)-C(10)	119.81(12)
C(12)-C(11)-C(10)	119.64(12)	O(1)-C(32)-N(31)	123.70(13)
C(15)-C(12)-C(11)	119.40(12)	O(1)-C(32)-C(34)	119.38(12)
C(15)-C(12)-C(13)	120.36(12)	N(31)-C(32)-C(34)	116.92(11)
C(11)-C(12)-C(13)	120.24(12)	N(35)-C(34)-C(47)	123.78(13)
C(12)-C(13)-C(14)	111.90(13)	N(35)-C(34)-C(32)	117.28(12)
C(12)-C(15)-C(26)	120.70(11)	C(47)-C(34)-C(32)	118.91(12)
C(12)-C(15)-C(16)	119.50(12)	C(34)-N(35)-C(36)	117.69(11)
C(26)-C(15)-C(16)	119.68(12)	N(35)-C(36)-C(45)	122.49(12)
N(17)-C(16)-C(15)	109.59(11)	N(35)-C(36)-C(37)	118.39(12)
C(18)-N(17)-C(16)	123.33(12)	C(45)-C(36)-C(37)	119.10(12)
N(25)-C(18)-N(17)	115.34(12)	N(38)-C(37)-C(42)	122.70(13)
N(25)-C(18)-C(19)	122.68(12)	N(38)-C(37)-C(36)	118.03(12)
N(17)-C(18)-C(19)	121.95(12)	C(42)-C(37)-C(36)	119.26(13)
C(20)-C(19)-C(18)	119.11(13)	C(39)-N(38)-C(37)	117.50(13)
C(19)-C(20)-C(22)	117.97(13)	N(38)-C(39)-C(40)	123.95(15)
C(19)-C(20)-C(21)	120.69(13)	C(41)-C(40)-C(39)	118.56(14)
C(22)-C(20)-C(21)	121.34(12)	C(40)-C(41)-C(42)	119.73(14)
C(23)-C(22)-C(20)	119.87(13)	C(41)-C(42)-C(37)	117.55(14)
N(25)-C(23)-C(22)	122.63(13)	C(41)-C(42)-C(43)	122.84(14)
N(25)-C(23)-C(24)	115.28(13)	C(37)-C(42)-C(43)	119.60(13)
C(22)-C(23)-C(24)	122.08(13)	C(44)-C(43)-C(42)	121.06(14)
C(18)-N(25)-C(23)	117.71(12)	C(43)-C(44)-C(45)	121.09(14)
C(15)-C(26)-C(29)	119.22(12)	C(46)-C(45)-C(36)	117.80(13)
C(15)-C(26)-C(27)	119.94(11)	C(46)-C(45)-C(44)	122.34(13)
C(29)-C(26)-C(27)	120.84(12)	C(36)-C(45)-C(44)	119.85(13)
C(26)-C(27)-C(28)	112.50(11)	C(47)-C(46)-C(45)	119.66(13)

C(48)-C(29)-C(26)	120.56(12)	C(46)-C(47)-C(34)	118.53(13)
C(48)-C(29)-C(30)	119.36(11)	C(29)-C(48)-C(11)	119.68(12)
C(26)-C(29)-C(30)	120.01(12)	C(29)-C(48)-C(49)	120.89(12)
N(31)-C(30)-C(29)	109.90(11)	C(11)-C(48)-C(49)	119.40(12)
C(32)-N(31)-C(30)	122.04(11)	C(48)-C(49)-C(50)	110.83(12)

Table 4. Torsion angles [°].

C(8)-N(1)-C(2)-C(4)	1.0(2)	N(17)-C(18)-N(25)-C(23)	179.82(13)
C(8)-N(1)-C(2)-C(3)	-178.52(12)	C(19)-C(18)-N(25)-C(23)	-1.8(2)
N(1)-C(2)-C(4)-C(5)	-0.5(2)	C(22)-C(23)-N(25)-C(18)	0.9(2)
C(3)-C(2)-C(4)-C(5)	178.95(14)	C(30)-N(31)-C(32)-C(34)	177.33(12)
C(2)-C(4)-C(5)-C(7)	0.2(2)	O(1)-C(32)-C(34)-N(35)	-160.23(13)
C(2)-C(4)-C(5)-C(6)	-176.99(14)	N(31)-C(32)-C(34)-N(35)	20.09(18)
C(4)-C(5)-C(7)-C(8)	-0.3(2)	O(1)-C(32)-C(34)-C(47)	17.9(2)
C(6)-C(5)-C(7)-C(8)	176.84(14)	N(31)-C(32)-C(34)-C(47)	-161.78(13)
C(2)-N(1)-C(8)-N(9)	179.79(12)	C(47)-C(34)-N(35)-C(36)	-1.9(2)
C(2)-N(1)-C(8)-C(7)	-1.12(19)	C(32)-C(34)-N(35)-C(36)	176.12(12)
C(5)-C(7)-C(8)-N(1)	0.8(2)	C(34)-N(35)-C(36)-C(45)	1.1(2)
C(5)-C(7)-C(8)-N(9)	179.87(13)	C(34)-N(35)-C(36)-C(37)	-177.64(12)
N(1)-C(8)-N(9)-C(10)	-8.29(19)	N(35)-C(36)-C(37)-N(38)	-2.78(19)
C(7)-C(8)-N(9)-C(10)	172.59(13)	C(45)-C(36)-C(37)-N(38)	178.46(12)
C(8)-N(9)-C(10)-C(11)	-172.05(12)	N(35)-C(36)-C(37)-C(42)	176.78(12)
N(9)-C(10)-C(11)-C(48)	-84.21(15)	C(45)-C(36)-C(37)-C(42)	-2.0(2)
N(9)-C(10)-C(11)-C(12)	90.50(15)	C(42)-C(37)-N(38)-C(39)	-0.7(2)
C(48)-C(11)-C(12)-C(15)	-1.02(19)	C(36)-C(37)-N(38)-C(39)	178.83(13)
C(10)-C(11)-C(12)-C(15)	-175.70(11)	C(37)-N(38)-C(39)-C(40)	0.4(2)
C(48)-C(11)-C(12)-C(13)	178.83(12)	N(38)-C(39)-C(40)-C(41)	0.1(2)
C(10)-C(11)-C(12)-C(13)	4.15(18)	C(39)-C(40)-C(41)-C(42)	-0.1(2)
C(15)-C(12)-C(13)-C(14)	-92.44(17)	C(40)-C(41)-C(42)-C(37)	-0.2(2)
C(11)-C(12)-C(13)-C(14)	87.71(17)	C(40)-C(41)-C(42)-C(43)	179.08(15)
C(11)-C(12)-C(15)-C(26)	3.44(18)	N(38)-C(37)-C(42)-C(41)	0.6(2)
C(13)-C(12)-C(15)-C(26)	-176.41(12)	C(36)-C(37)-C(42)-C(41)	-178.90(13)
C(11)-C(12)-C(15)-C(16)	179.57(11)	N(38)-C(37)-C(42)-C(43)	-178.66(13)
C(13)-C(12)-C(15)-C(16)	-0.28(18)	C(36)-C(37)-C(42)-C(43)	1.8(2)
C(12)-C(15)-C(16)-N(17)	-89.47(15)	C(41)-C(42)-C(43)-C(44)	-179.60(15)
C(26)-C(15)-C(16)-N(17)	86.70(15)	C(37)-C(42)-C(43)-C(44)	-0.3(2)
		C(42)-C(43)-C(44)-C(45)	-1.0(2)

C(15)-C(16)-N(17)-C(18)	-174.07(13)	N(35)-C(36)-C(45)-C(46)	0.9(2)
C(16)-N(17)-C(18)-N(25)	172.78(13)	C(37)-C(36)-C(45)-C(46)	179.63(13)
C(16)-N(17)-C(18)-C(19)	-5.6(2)	N(35)-C(36)-C(45)-C(44)	-177.99(13)
N(25)-C(18)-C(19)-C(20)	1.5(2)	C(37)-C(36)-C(45)-C(44)	0.7(2)
N(17)-C(18)-C(19)-C(20)	179.82(14)	C(43)-C(44)-C(45)-C(46)	-178.10(14)
C(18)-C(19)-C(20)-C(22)	-0.4(2)	C(43)-C(44)-C(45)-C(36)	0.8(2)
C(18)-C(19)-C(20)-C(21)	179.14(13)	C(36)-C(45)-C(46)-C(47)	-2.2(2)
C(19)-C(20)-C(22)-C(23)	-0.4(2)	C(44)-C(45)-C(46)-C(47)	176.72(14)
C(21)-C(20)-C(22)-C(23)	-179.93(14)	C(45)-C(46)-C(47)-C(34)	1.4(2)
C(20)-C(22)-C(23)-N(25)	0.2(2)	N(35)-C(34)-C(47)-C(46)	0.7(2)
C(20)-C(22)-C(23)-C(24)	179.09(14)	C(32)-C(34)-C(47)-C(46)	-177.33(13)
C(24)-C(23)-N(25)-C(18)	-178.07(13)	C(26)-C(29)-C(48)-C(11)	0.32(19)
C(12)-C(15)-C(26)-C(29)	-3.95(18)	C(30)-C(29)-C(48)-C(11)	-176.55(12)
C(16)-C(15)-C(26)-C(29)	179.93(11)	C(26)-C(29)-C(48)-C(49)	-177.66(12)
C(12)-C(15)-C(26)-C(27)	176.19(12)	C(30)-C(29)-C(48)-C(49)	5.47(18)
C(16)-C(15)-C(26)-C(27)	0.07(18)	C(12)-C(11)-C(48)-C(29)	-0.84(19)
C(15)-C(26)-C(27)-C(28)	90.44(15)	C(10)-C(11)-C(48)-C(29)	173.83(11)
C(29)-C(26)-C(27)-C(28)	-89.42(15)	C(12)-C(11)-C(48)-C(49)	177.17(11)
C(15)-C(26)-C(29)-C(48)	2.05(18)	C(10)-C(11)-C(48)-C(49)	-8.16(18)
C(27)-C(26)-C(29)-C(48)	-178.09(12)	C(29)-C(48)-C(49)-C(50)	93.12(15)
C(15)-C(26)-C(29)-C(30)	178.90(11)	C(11)-C(48)-C(49)-C(50)	-84.87(16)
C(27)-C(26)-C(29)-C(30)	-1.25(18)		
C(48)-C(29)-C(30)-N(31)	79.76(15)		
C(26)-C(29)-C(30)-N(31)	-97.13(14)		
C(29)-C(30)-N(31)-C(32)	-138.74(13)		
C(30)-N(31)-C(32)-O(1)	-2.3(2)		