Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting information

Glycosyl nitrates in synthesis: streamlined access to glucopyranose building blocks differentiated at C-2

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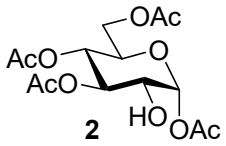

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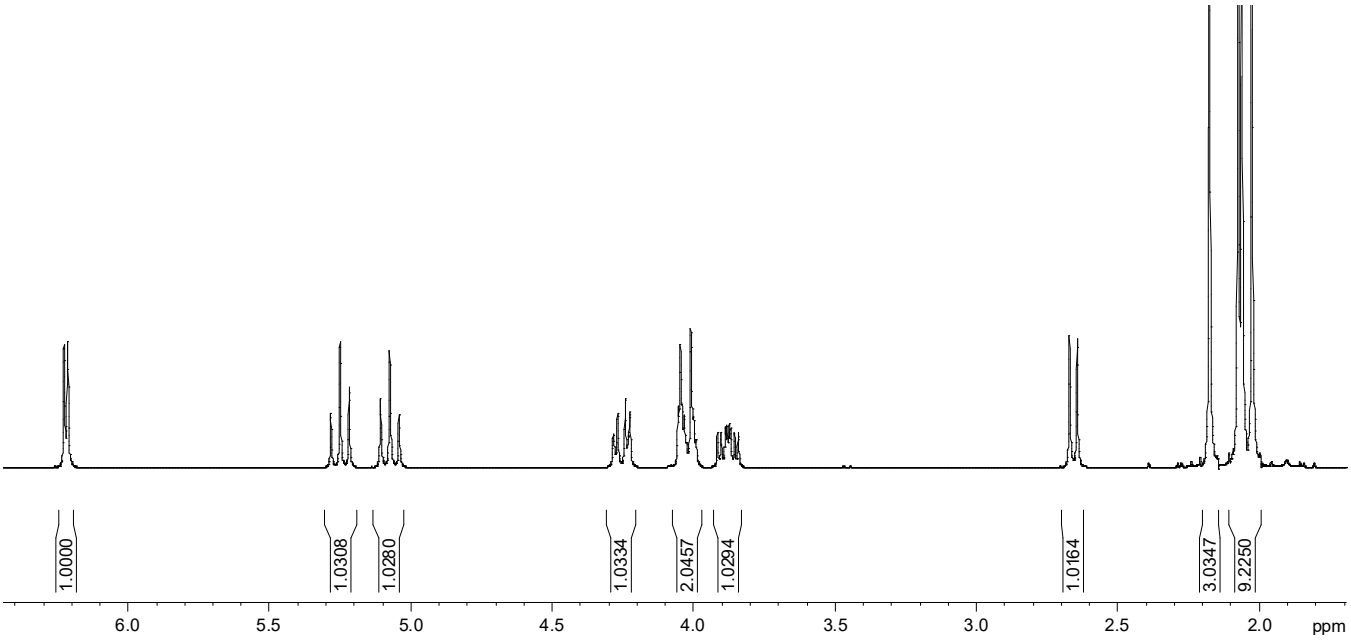

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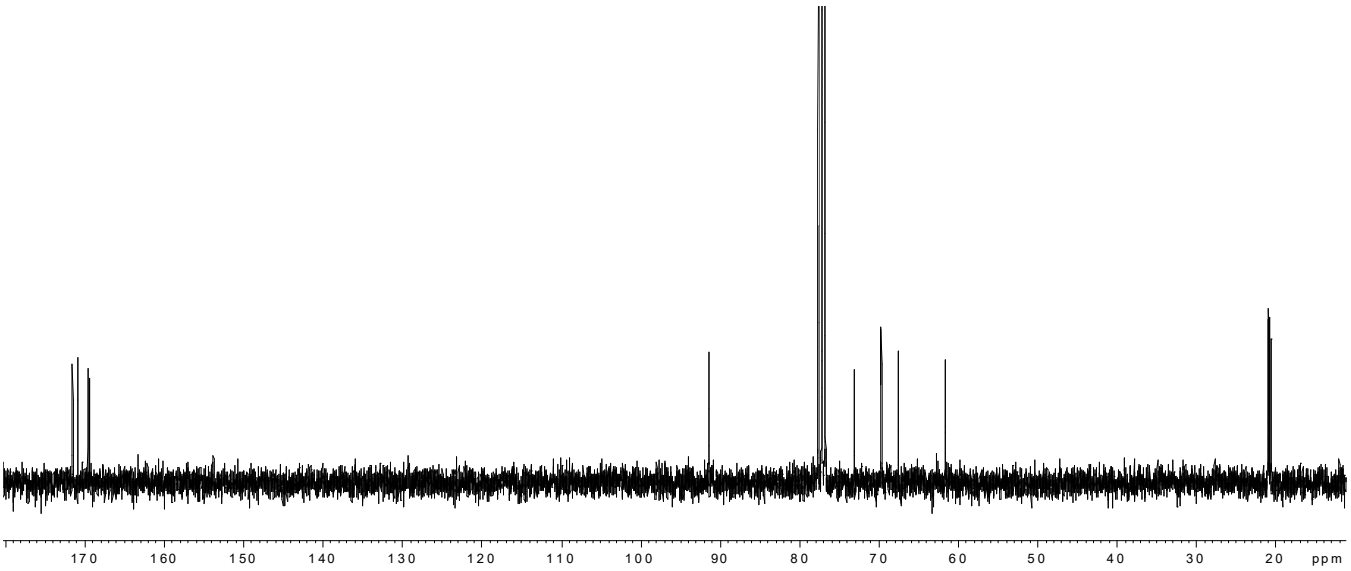

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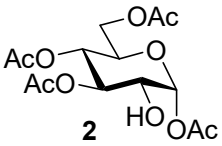

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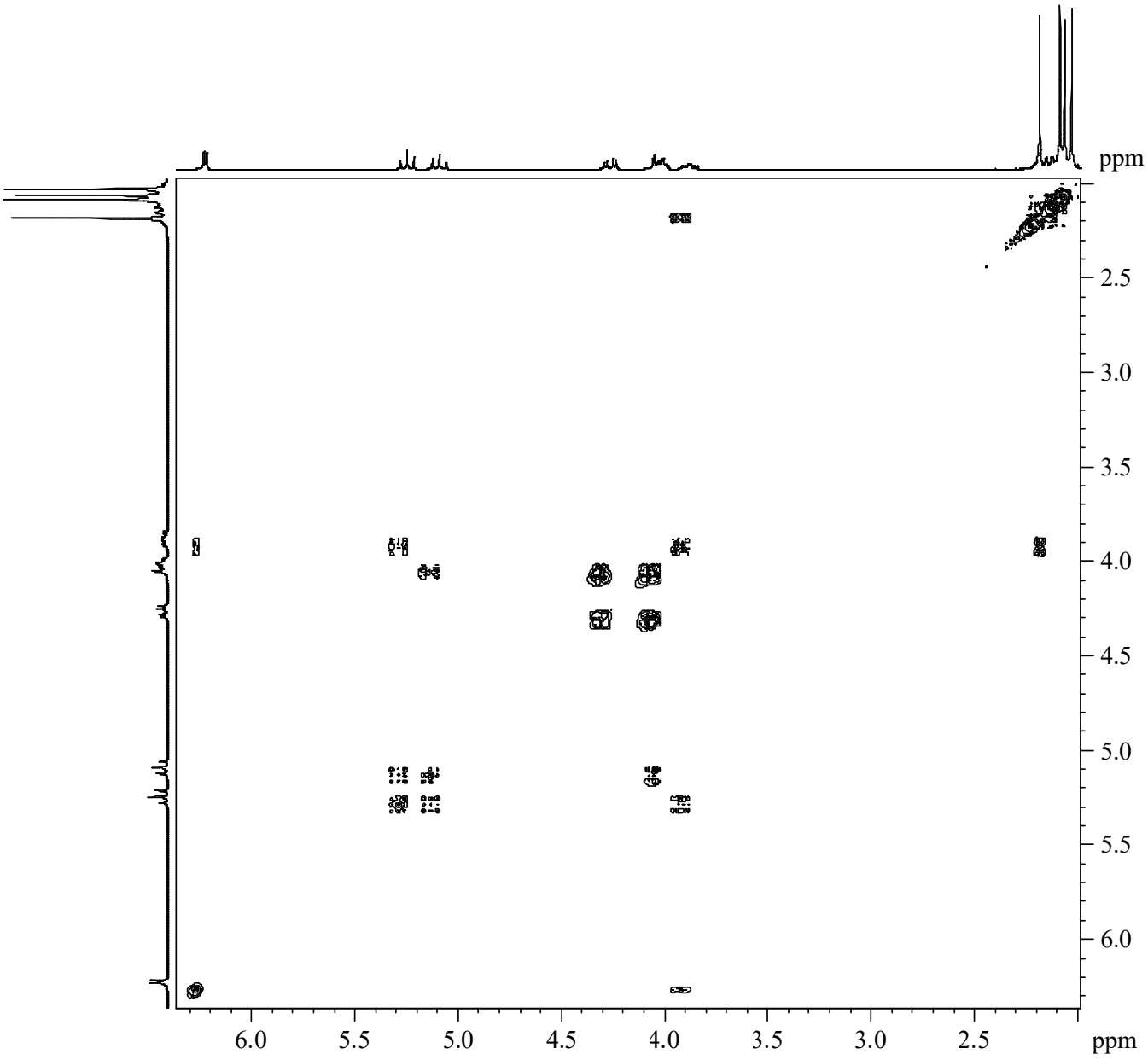

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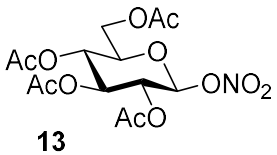

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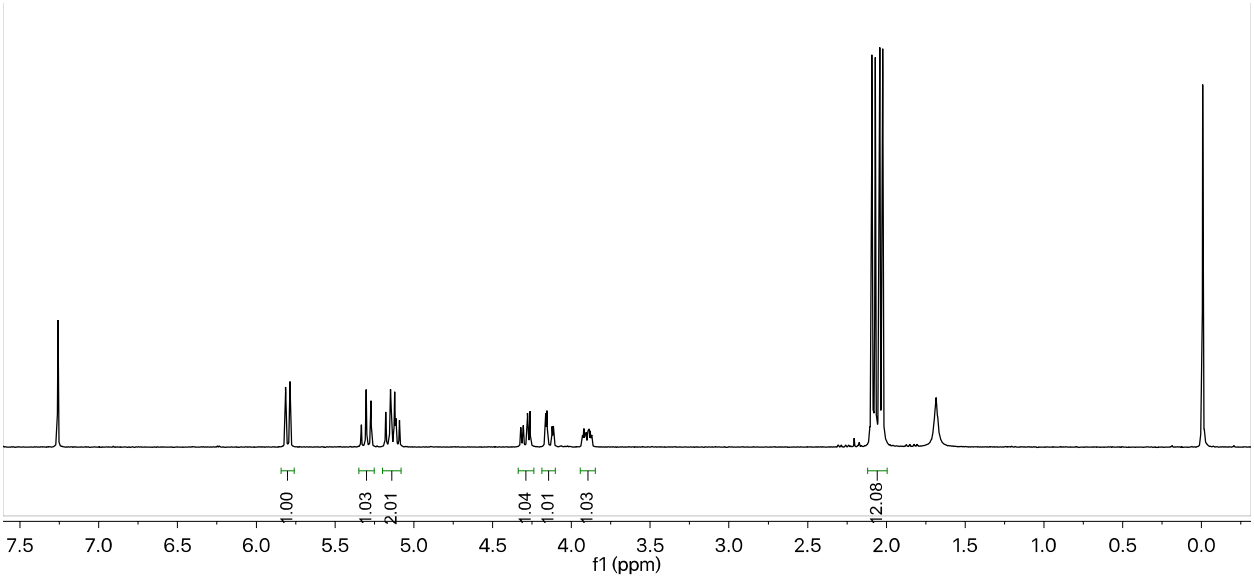

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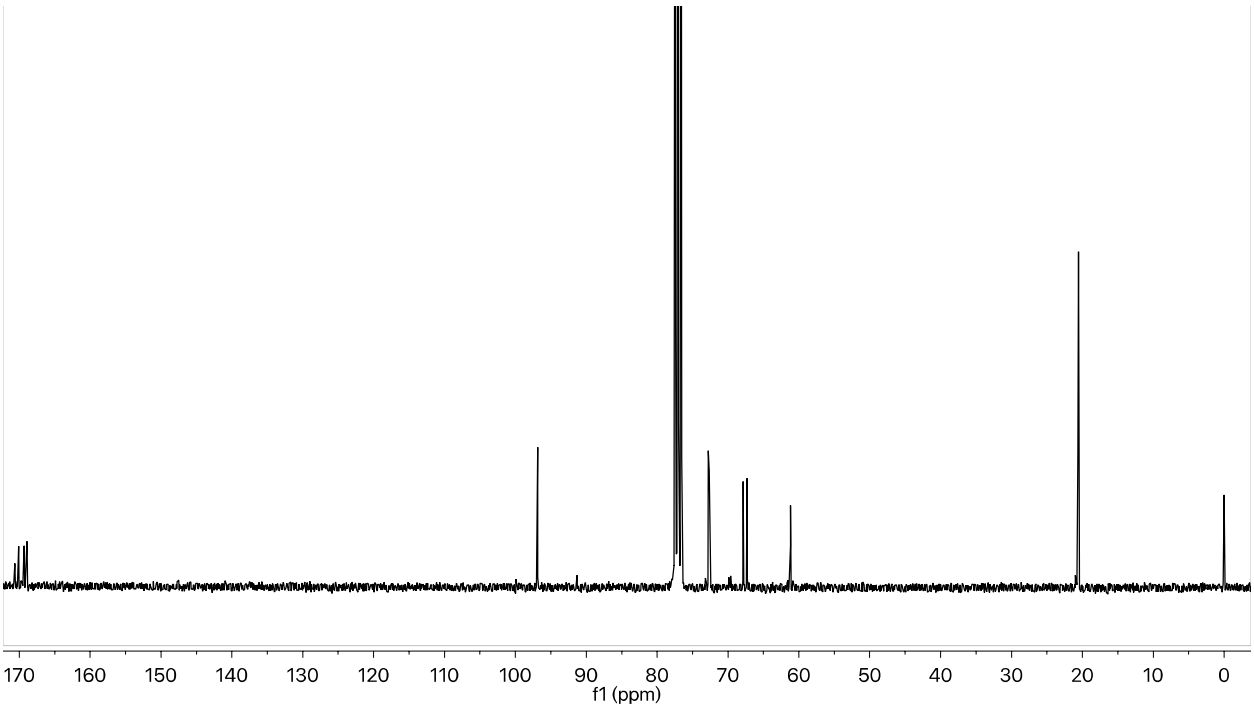

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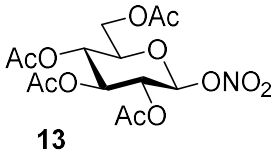

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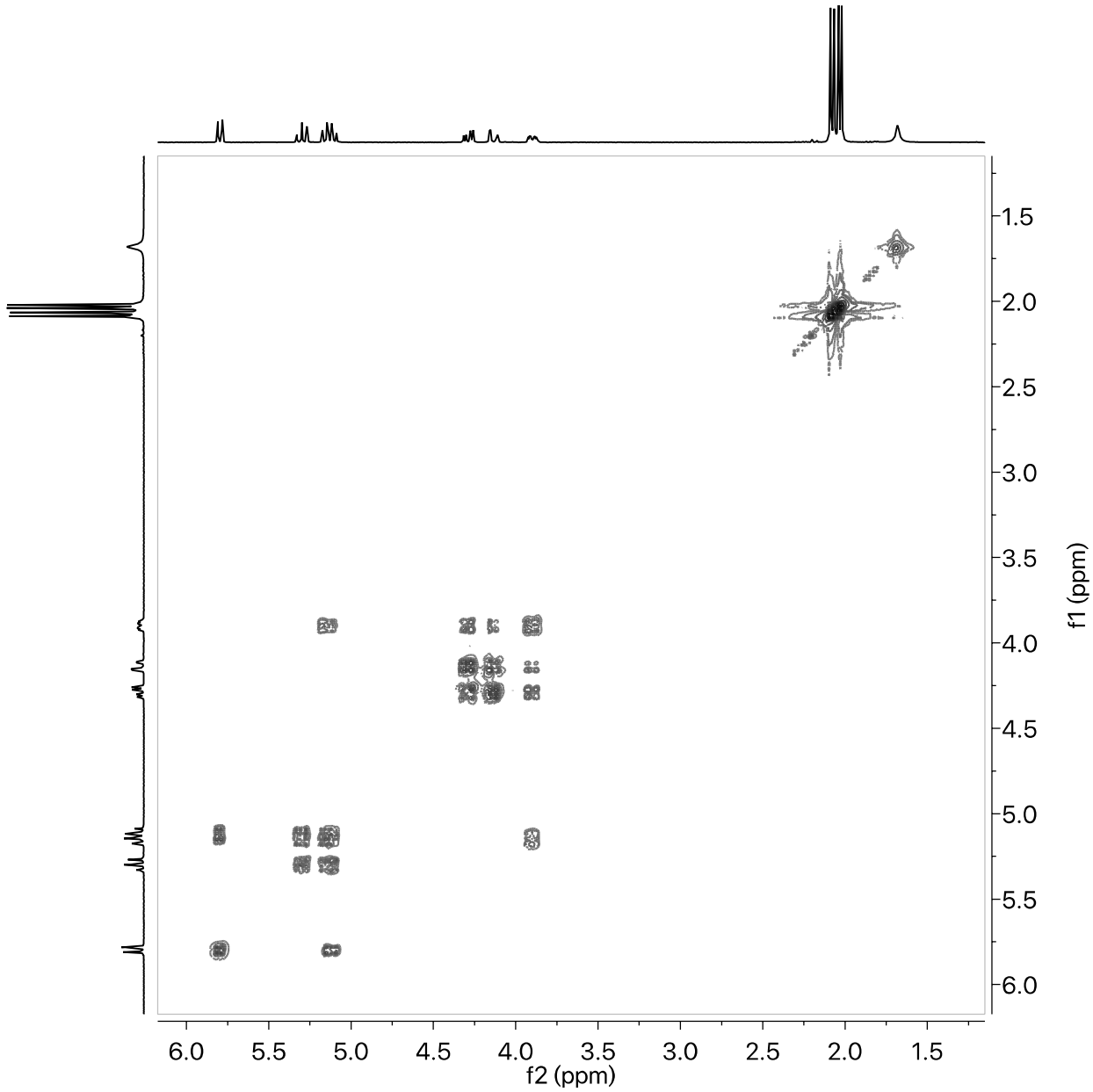

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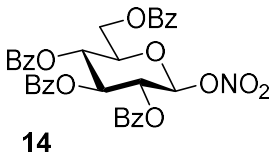

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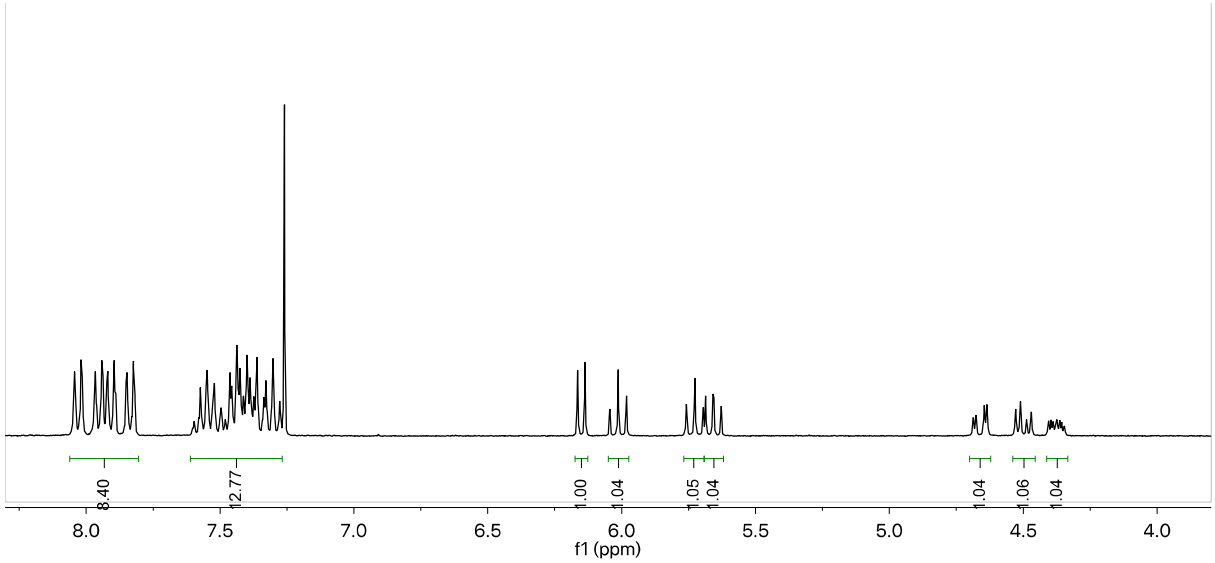

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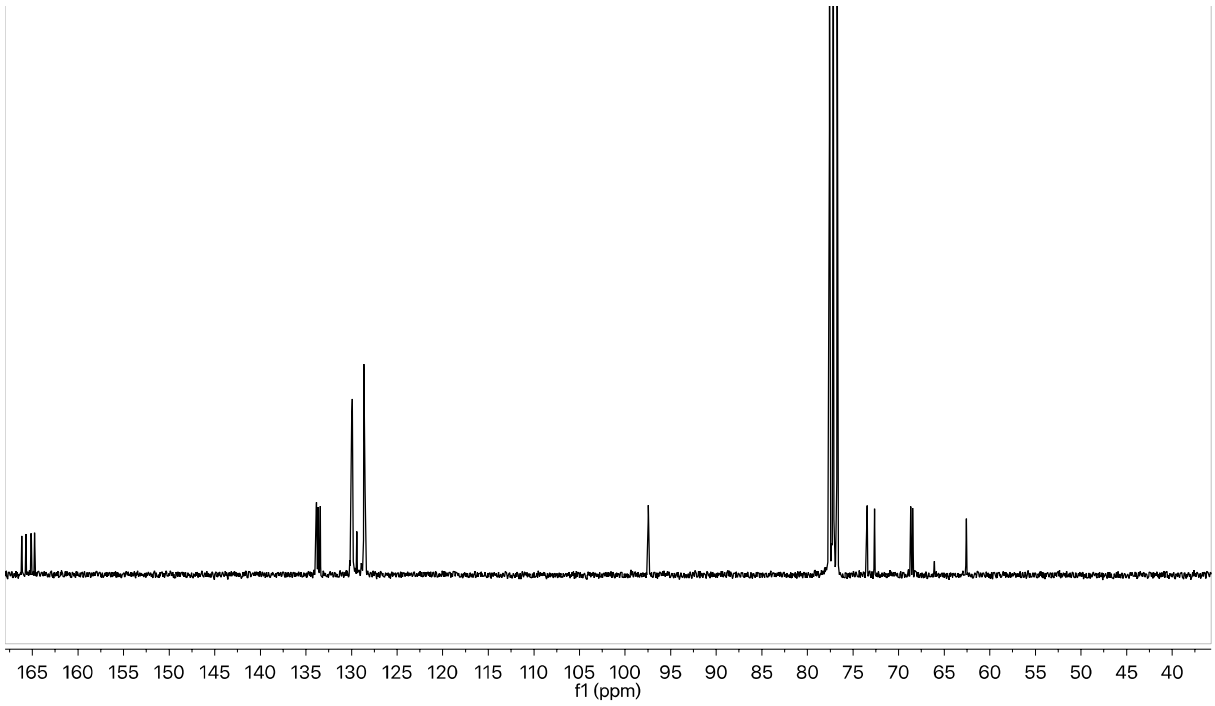

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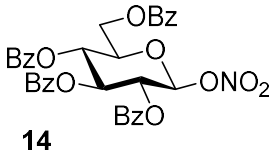

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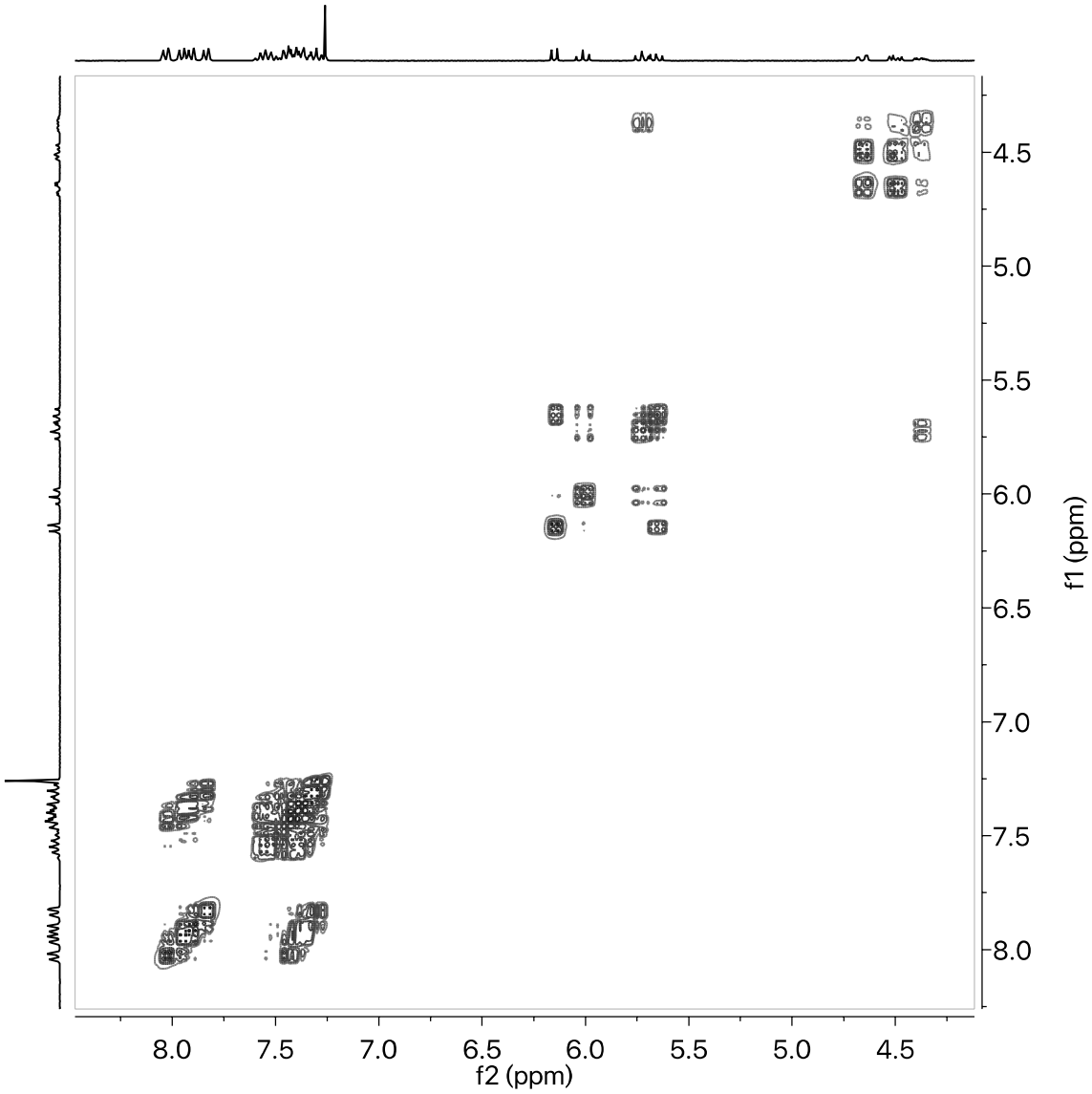

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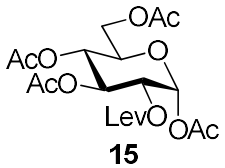

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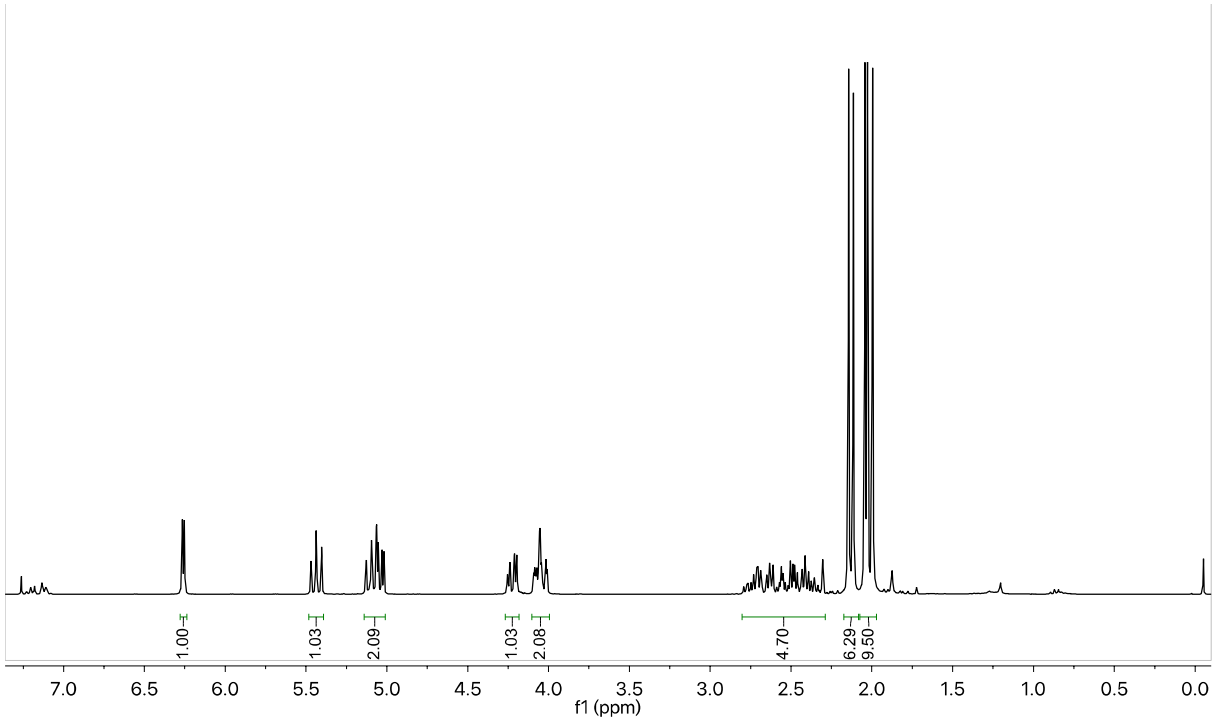

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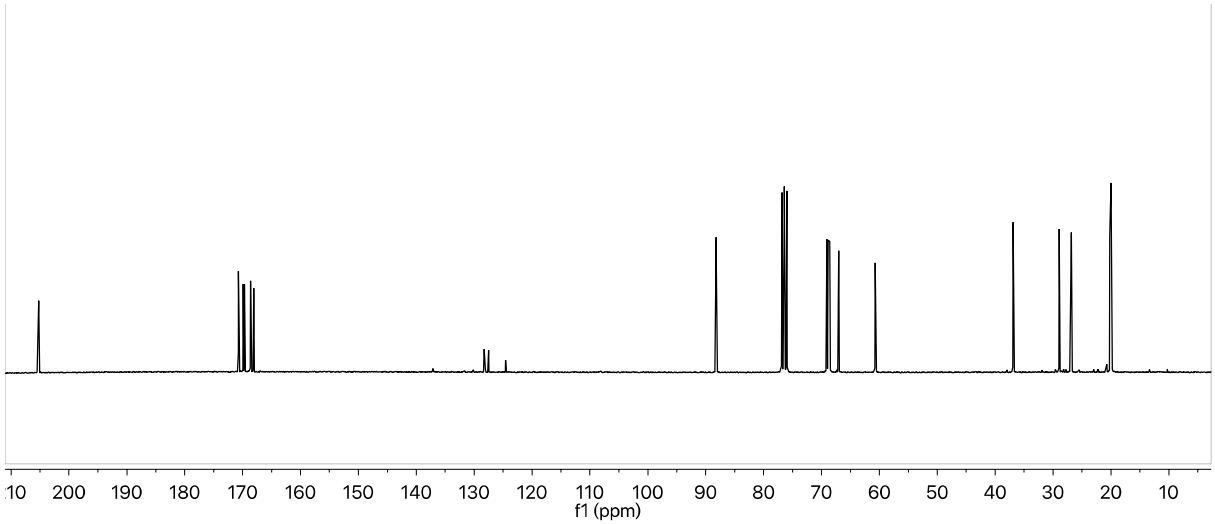

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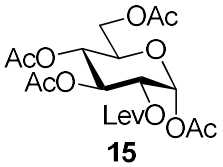

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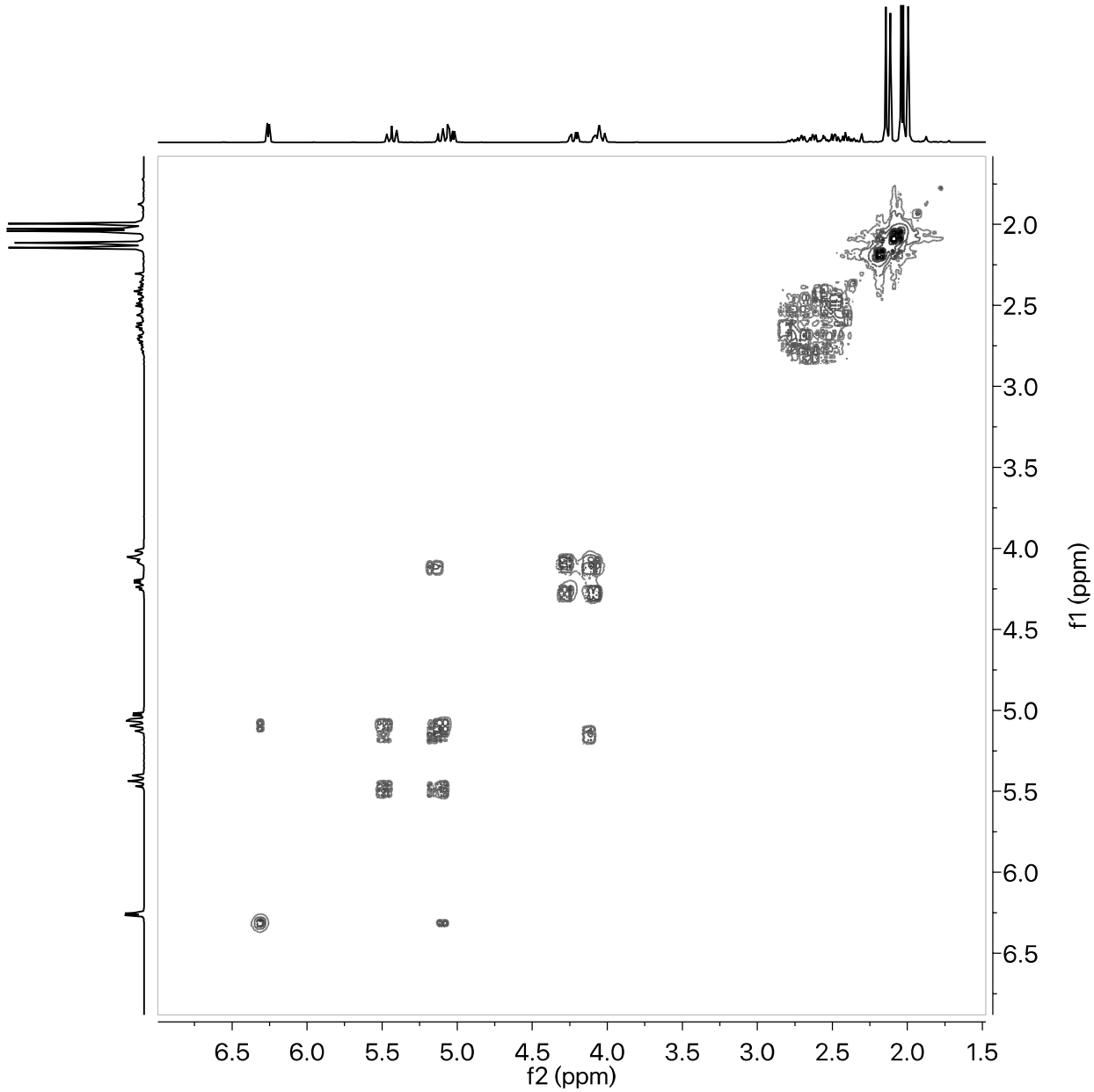

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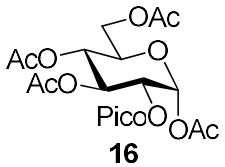

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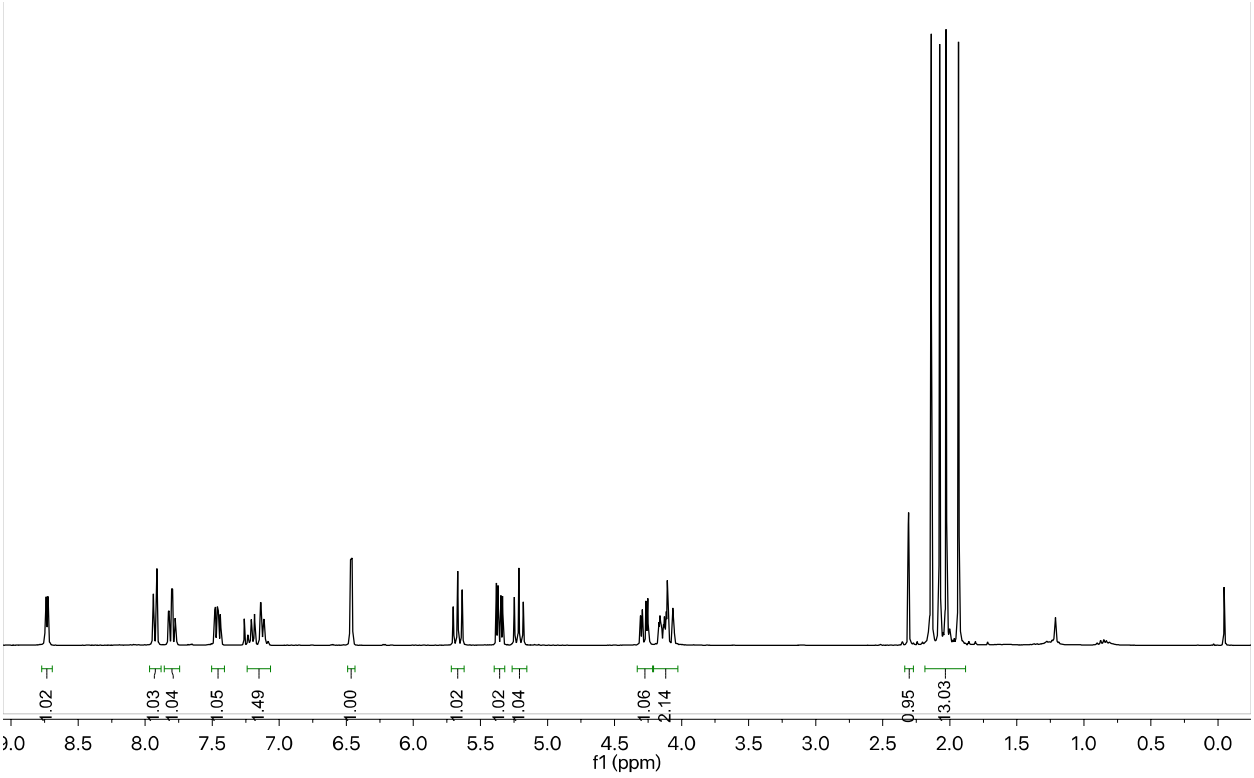

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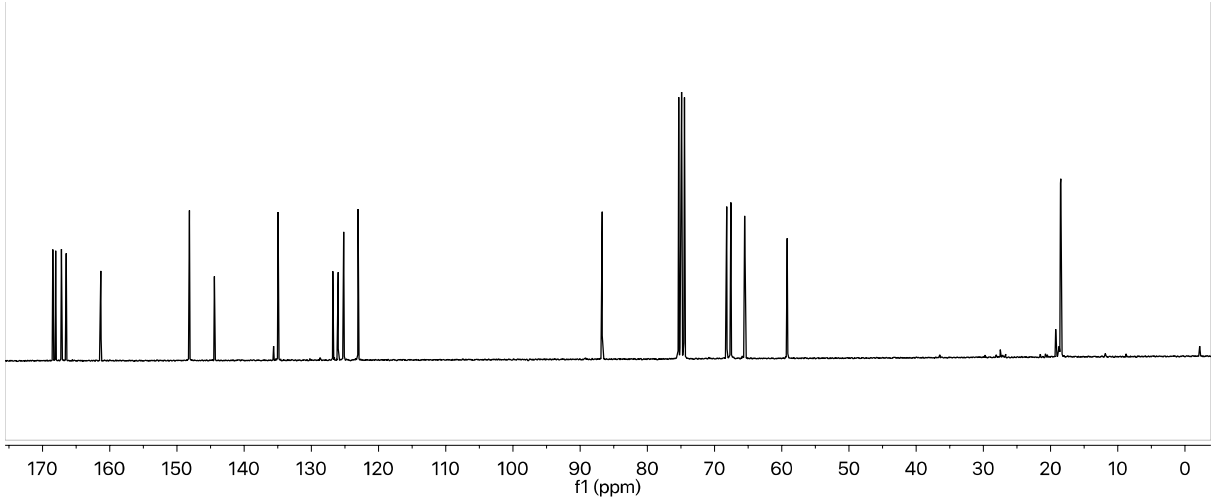
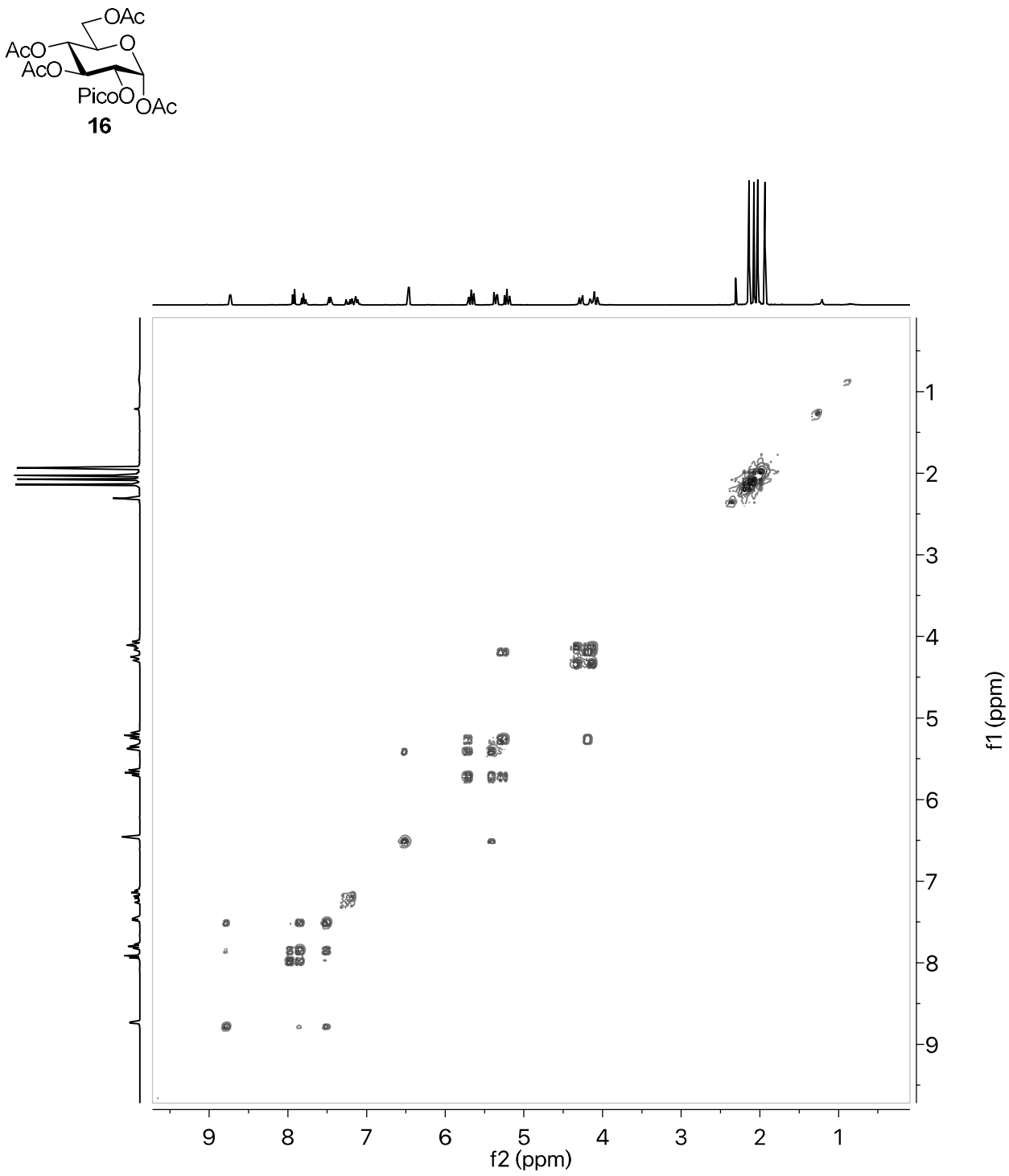


(^{13}C NMR 75 MHz, $CDCl_3$)



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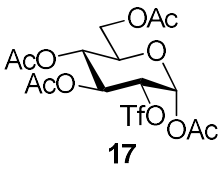

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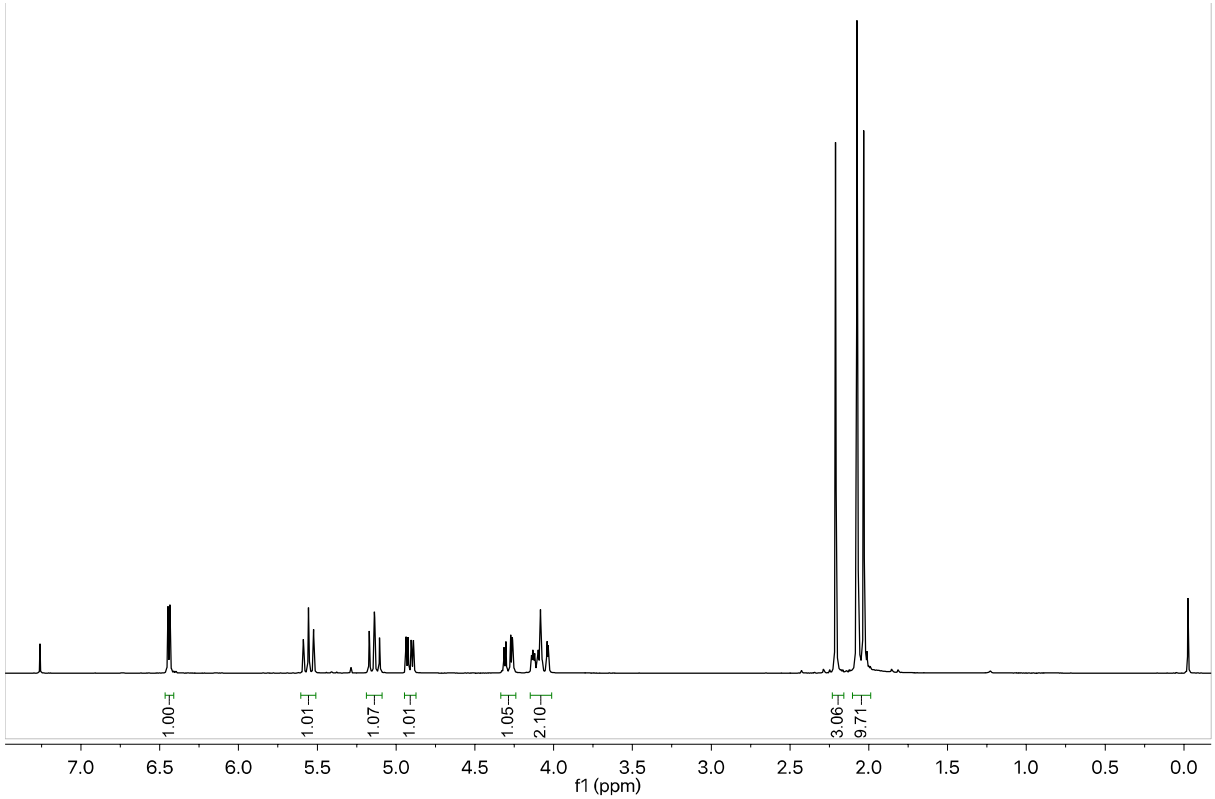

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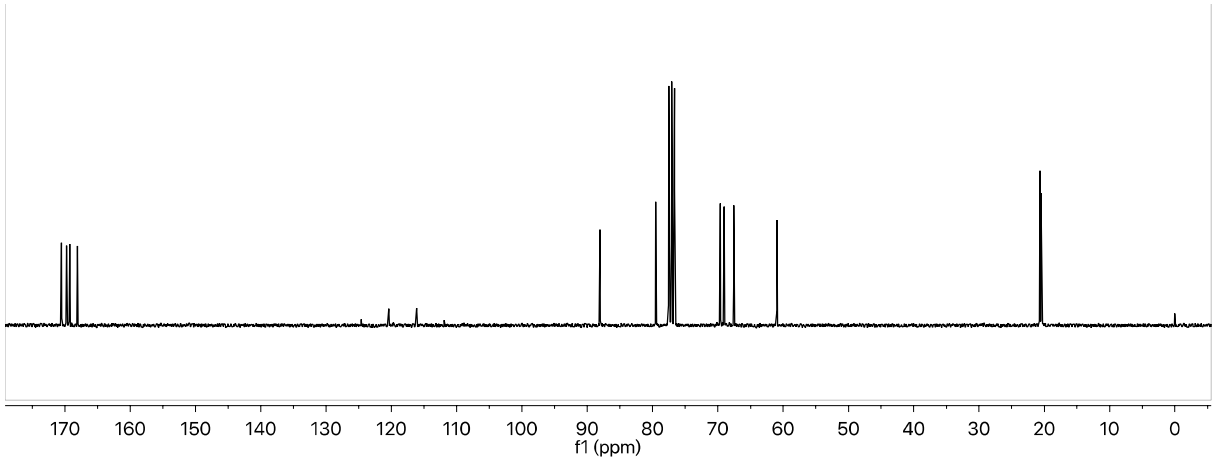

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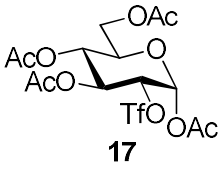

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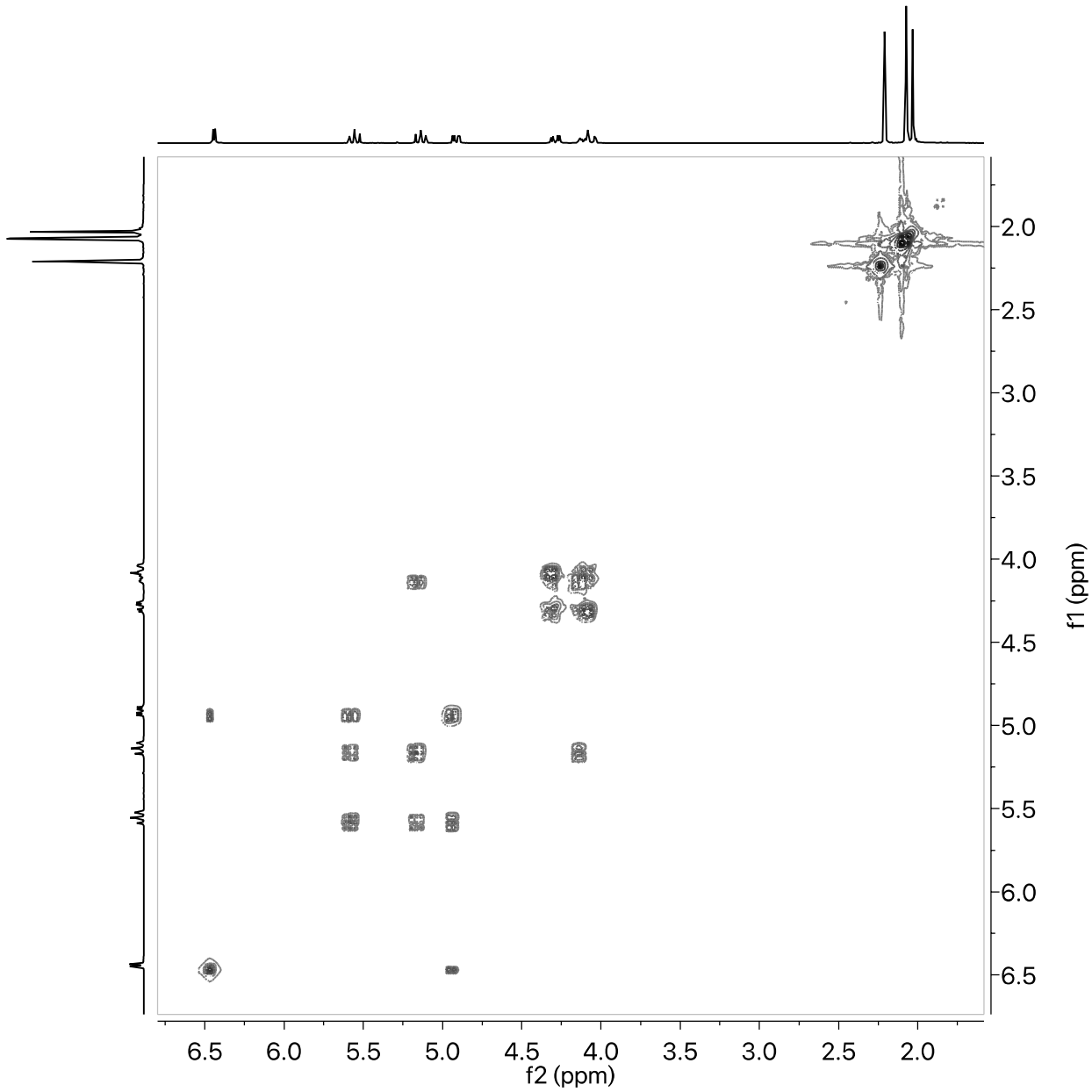

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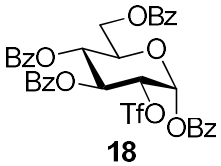

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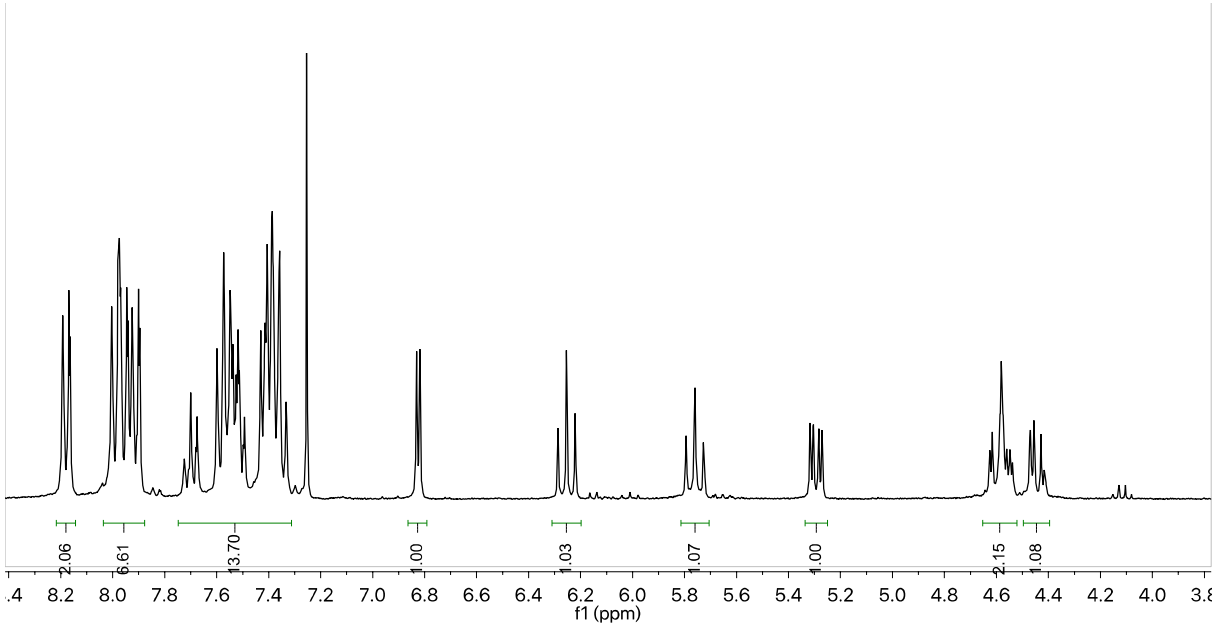
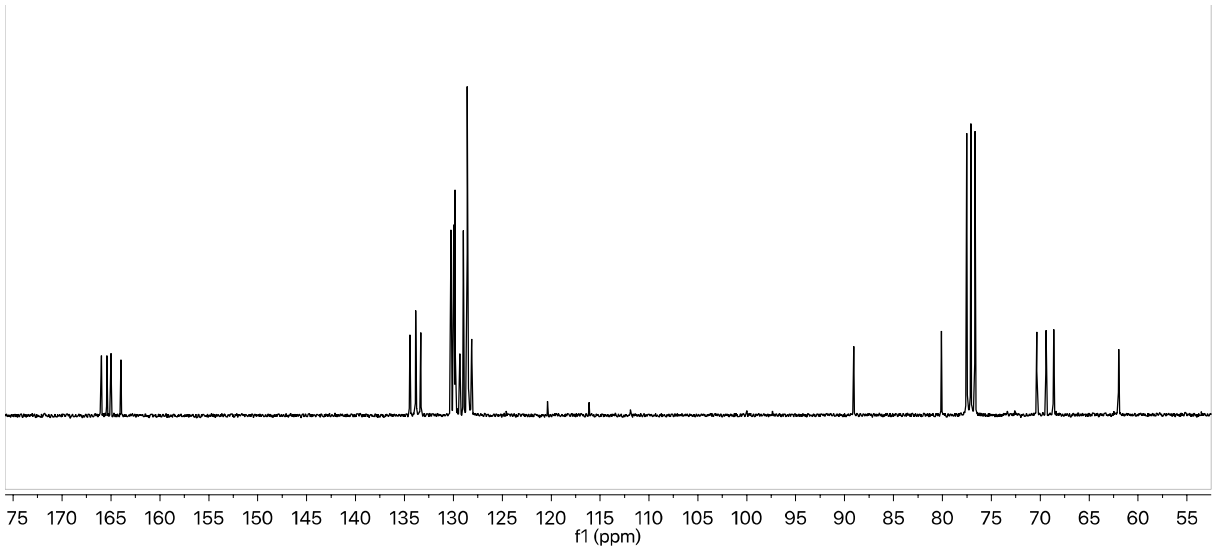
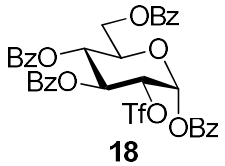


(^{1}H NMR 300 MHz, $CDCl_3$)



(^{13}C NMR 75 MHz, $CDCl_3$)



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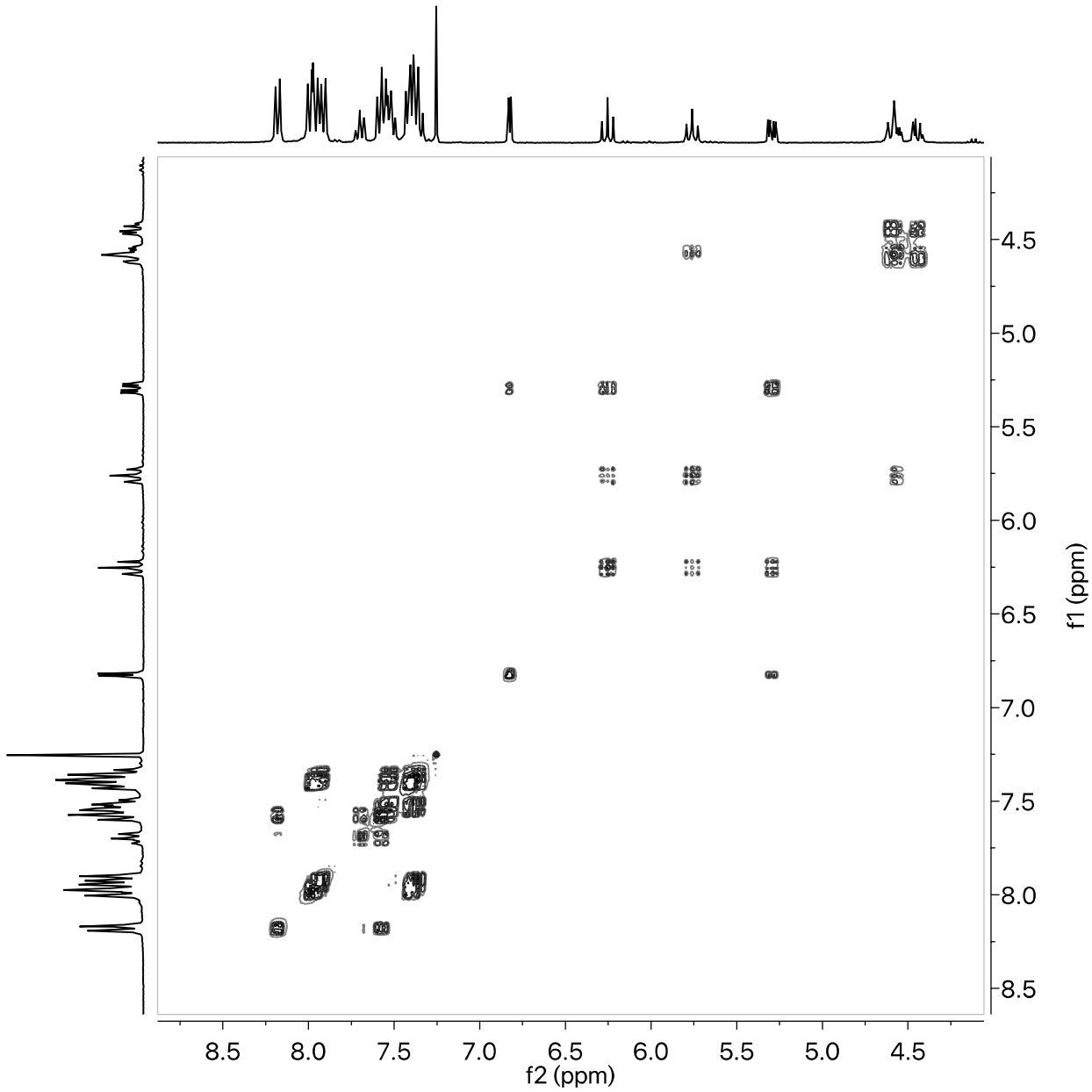
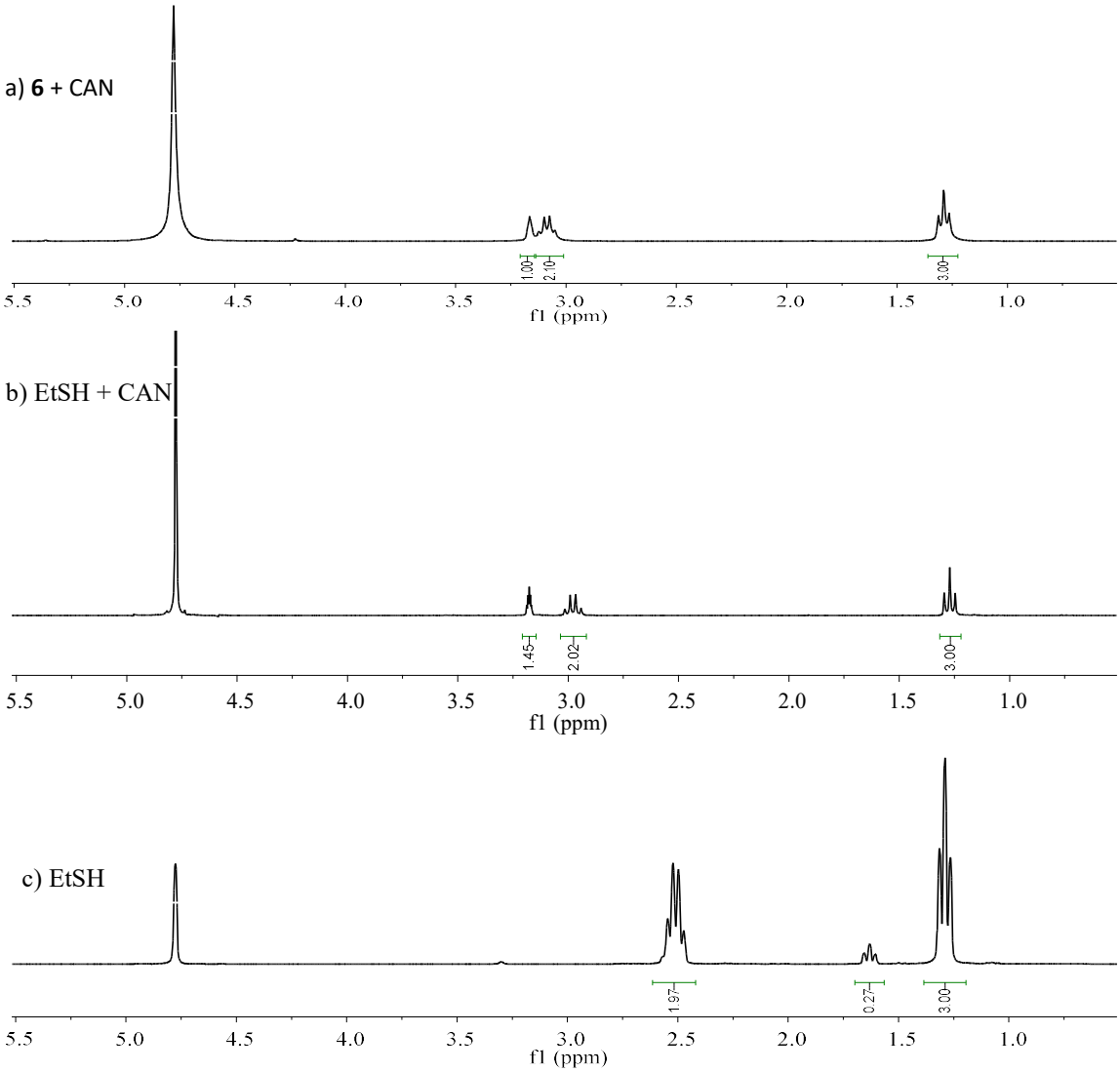


(2D NMR 300 MHz, $CDCl_3$)

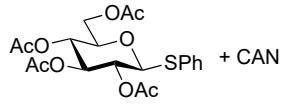
NMR Spectra: a) White Precipitate from CAN Reaction with thioglycoside **6**; b) White Precipitate from CAN Reaction of Ethanethiol; c) Pure Ethanethiol

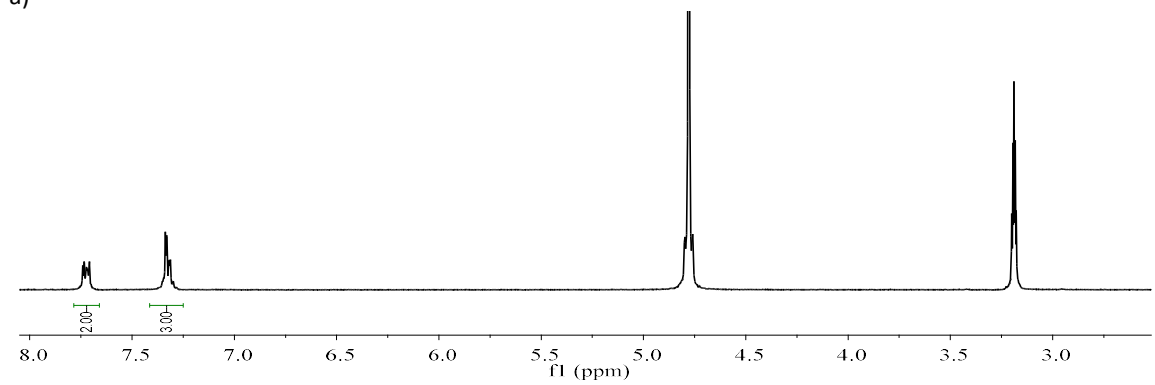


(^{1}H NMR 300 MHz, CD_3OD)

NMR Spectra: a) ^{1}H Spectrum of White Precipitate from CAN Reaction of SPh Glycoside **11**; b) Pure Thiophenol; c) ^{13}C Spectrum of White Precipitate from CAN Reaction of SPh Glycoside **11**

a)





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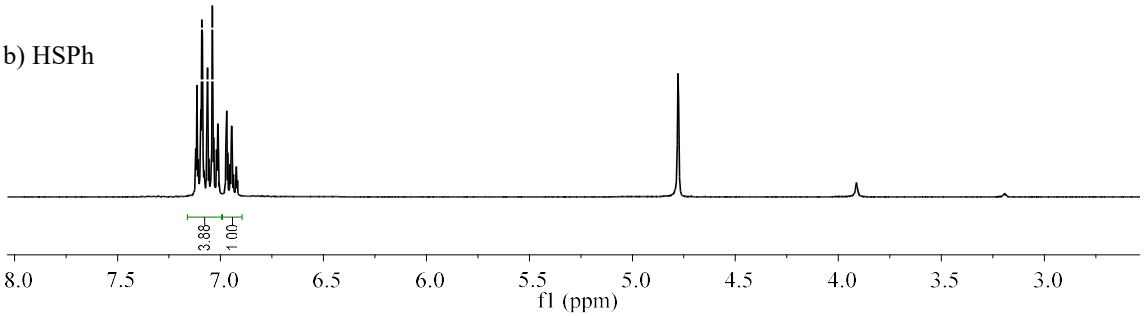
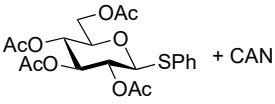
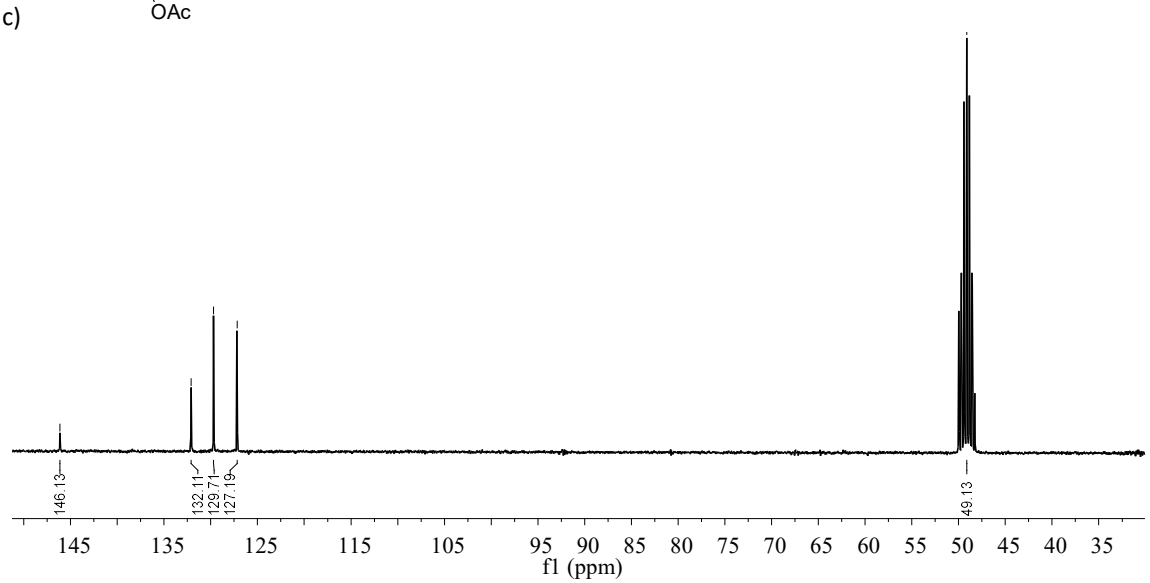


(^{1}H NMR 300 MHz, CD_3OD)

c)





(^{13}C NMR 75 MHz, $CDCl_3$)

X-Ray data

Compound 10

Table 1S. Crystal data and structure refinement for **10**.

Identification code	a16316t5/lt/smart/TB4-P132-2/	
Empirical formula	$Ce\ H_{16}\ N_7\ O_{19}$	
Formula weight	558.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 11.0806(4) Å	α= 90°.
	b = 8.8522(4) Å	β= 102.8202(18)°.
	c = 17.7829(6) Å	γ = 90°.
Volume	1700.80(11) $Å^3$	
Z	4	
Density (calculated)	2.180 Mg/m^3	
Absorption coefficient	2.790 mm^{-1}	
F(000)	1100	
Crystal size	0.229 x 0.118 x 0.075 mm^3	
Theta range for data collection	2.349 to 36.304°.	
Index ranges	$-18\leq h\leq 18$, $0\leq k\leq 14$, $0\leq l\leq 29$	
Reflections collected	27155	
Independent reflections	4419 [R(int) = 0.051]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.438258 and 0.344314	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4419 / 10 / 164	
Goodness-of-fit on F^2	1.161	
Final R indices [I>2sigma(I)]	R1 = 0.0440, wR2 = 0.1119	
R indices (all data)	R1 = 0.0516, wR2 = 0.1151	
Largest diff. peak and hole	1.057 and -1.251 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Ce(1)	5000	5615(1)	7500	9(1)
O(1)	5801(3)	7526(4)	8618(2)	22(1)
O(2)	3918(3)	7975(4)	8006(2)	21(1)
O(3)	4816(10)	9525(9)	8902(6)	24(1)
O(3')	4656(7)	9091(8)	9128(4)	24(1)
O(4)	4126(3)	4155(4)	6180(2)	20(1)
O(5)	5963(3)	5082(4)	6291(2)	23(1)
O(6)	5131(10)	3871(10)	5249(4)	19(2)
O(6')	5288(7)	3272(10)	5427(4)	32(2)
O(9)	7357(2)	5588(3)	7924(2)	14(1)
N(1)	4819(3)	8273(5)	8573(2)	29(1)
N(2)	5108(4)	4242(6)	5921(2)	28(1)
N(3)	5000	2094(4)	7500	17(1)
O(7)	4061(12)	2810(7)	7584(18)	18(1)
O(8)	4770(6)	762(6)	7248(4)	22(1)
O(7')	5929(12)	2812(7)	7395(18)	18(1)
O(1S)	6898(8)	1370(10)	5422(5)	26(2)
N(4)	2620(7)	1748(9)	5552(4)	21(2)
O(1S')	7091(8)	1005(11)	5188(6)	18(2)
N(4')	2922(8)	967(12)	5610(5)	17(2)

Table 3S. Bond lengths [Å] and angles [°] for **10**.

Ce(1)-O(9)	2.553(3)	O(1)-Ce(1)-O(5)#1	68.10(11)
Ce(1)-O(9)#1	2.553(3)	O(1)#1-Ce(1)-O(5)#1	127.13(10)
Ce(1)-O(1)	2.611(3)	O(9)-Ce(1)-O(5)	70.58(9)
Ce(1)-O(1)#1	2.611(3)	O(9)#1-Ce(1)-O(5)	109.22(9)
Ce(1)-O(5)#1	2.646(3)	O(1)-Ce(1)-O(5)	127.14(11)
Ce(1)-O(5)	2.646(3)	O(1)#1-Ce(1)-O(5)	68.10(11)
Ce(1)-O(2)#1	2.663(3)	O(5)#1-Ce(1)-O(5)	159.48(17)
Ce(1)-O(2)	2.663(3)	O(9)-Ce(1)-O(2)#1	66.38(9)
Ce(1)-O(4)#1	2.667(3)	O(9)#1-Ce(1)-O(2)#1	114.53(9)
Ce(1)-O(4)	2.667(3)	O(1)-Ce(1)-O(2)#1	69.30(11)
Ce(1)-O(7')	2.708(6)	O(1)#1-Ce(1)-O(2)#1	48.45(9)
Ce(1)-O(7)	2.709(6)	O(5)#1-Ce(1)-O(2)#1	135.01(11)
O(1)-N(1)	1.261(4)	O(5)-Ce(1)-O(2)#1	64.67(11)
O(2)-N(1)	1.278(4)	O(9)-Ce(1)-O(2)	114.53(9)
O(3)-N(1)	1.254(7)	O(9)#1-Ce(1)-O(2)	66.38(9)
O(3')-N(1)	1.269(6)	O(1)-Ce(1)-O(2)	48.45(8)
O(4)-N(2)	1.275(5)	O(1)#1-Ce(1)-O(2)	69.30(11)
O(5)-N(2)	1.268(5)	O(5)#1-Ce(1)-O(2)	64.67(11)
O(6)-N(2)	1.244(6)	O(5)-Ce(1)-O(2)	135.01(11)
O(6')-N(2)	1.274(6)	O(2)#1-Ce(1)-O(2)	76.62(15)
O(9)-H(9A)	0.8857	O(9)-Ce(1)-O(4)#1	65.67(9)
O(9)-H(9B)	0.8860	O(9)#1-Ce(1)-O(4)#1	113.77(9)
N(3)-O(7)	1.255(6)	O(1)-Ce(1)-O(4)#1	69.39(11)
N(3)-O(7')	1.259(6)	O(1)#1-Ce(1)-O(4)#1	168.50(10)
N(3)-O(8)	1.267(5)	O(5)#1-Ce(1)-O(4)#1	48.04(9)
		O(5)-Ce(1)-O(4)#1	119.74(10)
O(9)-Ce(1)-O(9)#1	178.94(13)	O(2)#1-Ce(1)-O(4)#1	125.12(9)
O(9)-Ce(1)-O(1)	68.20(9)	O(2)-Ce(1)-O(4)#1	100.68(10)
O(9)#1-Ce(1)-O(1)	112.54(9)	O(9)-Ce(1)-O(4)	113.77(9)
O(9)-Ce(1)-O(1)#1	112.54(9)	O(9)#1-Ce(1)-O(4)	65.67(9)
O(9)#1-Ce(1)-O(1)#1	68.20(9)	O(1)-Ce(1)-O(4)	168.50(10)
O(1)-Ce(1)-O(1)#1	99.24(15)	O(1)#1-Ce(1)-O(4)	69.39(11)
O(9)-Ce(1)-O(5)#1	109.22(9)	O(5)#1-Ce(1)-O(4)	119.74(10)
O(9)#1-Ce(1)-O(5)#1	70.58(9)	O(5)-Ce(1)-O(4)	48.03(9)

O(2)#1-Ce(1)-O(4)	100.68(10)	O(7')-Ce(1)-O(7)	47.22(12)
O(2)-Ce(1)-O(4)	125.12(9)	N(1)-O(1)-Ce(1)	98.6(2)
O(4)#1-Ce(1)-O(4)	122.02(15)	N(1)-O(2)-Ce(1)	95.6(2)
O(9)-Ce(1)-O(7')	68.4(3)	N(2)-O(4)-Ce(1)	96.7(2)
O(9)#1-Ce(1)-O(7')	110.5(3)	N(2)-O(5)-Ce(1)	97.9(2)
O(1)-Ce(1)-O(7')	125.2(6)	Ce(1)-O(9)-H(9A)	110.1
O(1)#1-Ce(1)-O(7')	127.7(7)	Ce(1)-O(9)-H(9B)	110.2
O(5)#1-Ce(1)-O(7')	96.9(5)	H(9A)-O(9)-H(9B)	108.7
O(5)-Ce(1)-O(7')	63.4(5)	O(3)-N(1)-O(1)	121.7(6)
O(2)#1-Ce(1)-O(7')	119.3(3)	O(1)-N(1)-O(3')	121.3(4)
O(2)-Ce(1)-O(7')	161.5(5)	O(3)-N(1)-O(2)	117.9(6)
O(4)#1-Ce(1)-O(7')	63.1(7)	O(1)-N(1)-O(2)	117.0(3)
O(4)-Ce(1)-O(7')	64.2(7)	O(3')-N(1)-O(2)	120.7(4)
O(9)-Ce(1)-O(7)	110.8(3)	O(6)-N(2)-O(5)	118.8(6)
O(9)#1-Ce(1)-O(7)	68.1(3)	O(5)-N(2)-O(6')	122.7(5)
O(1)-Ce(1)-O(7)	128.4(7)	O(6)-N(2)-O(4)	122.1(6)
O(1)#1-Ce(1)-O(7)	124.5(6)	O(5)-N(2)-O(4)	116.6(3)
O(5)#1-Ce(1)-O(7)	64.1(5)	O(6')-N(2)-O(4)	119.0(5)
O(5)-Ce(1)-O(7)	96.4(5)	O(7)-N(3)-O(7')	119.3(4)
O(2)#1-Ce(1)-O(7)	160.9(5)	O(7)-N(3)-O(8)	113.9(7)
O(2)-Ce(1)-O(7)	119.6(2)	O(7')-N(3)-O(8)	121.6(7)
O(4)#1-Ce(1)-O(7)	64.9(7)	N(3)-O(7)-Ce(1)	96.7(4)
O(4)-Ce(1)-O(7)	62.3(7)	N(3)-O(7')-Ce(1)	96.7(4)

Symmetry transformations used to generate equivalent atoms:

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

Table 4S. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **10**. 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}
Ce(1)	9(1)	7(1)	11(1)	0	2(1)	0
O(1)	12(1)	19(1)	30(2)	-8(1)	-4(1)	6(1)
O(2)	12(1)	18(1)	28(1)	-8(1)	-6(1)	3(1)
O(3)	28(2)	17(3)	23(3)	-6(2)	-3(2)	10(2)
O(3')	28(2)	17(3)	23(3)	-6(2)	-3(2)	10(2)
O(4)	14(1)	26(2)	20(1)	-5(1)	4(1)	-3(1)
O(5)	16(1)	34(2)	18(1)	-5(1)	5(1)	-5(1)
O(6)	38(5)	9(3)	10(3)	2(2)	6(3)	5(3)
O(6')	39(3)	36(4)	24(3)	-15(3)	11(3)	7(3)
O(9)	10(1)	10(1)	22(1)	2(1)	4(1)	0(1)
N(1)	19(2)	25(2)	35(2)	-18(2)	-9(1)	11(1)
N(2)	20(2)	47(3)	18(1)	-15(2)	6(1)	-5(2)
N(3)	20(2)	6(2)	27(2)	0	12(2)	0
O(7)	14(1)	13(1)	28(2)	-6(8)	7(1)	-8(6)
O(8)	28(3)	10(2)	32(3)	-7(2)	13(2)	-7(2)
O(7')	14(1)	13(1)	28(2)	-6(8)	7(1)	-8(6)
O(1S)	33(3)	21(3)	25(3)	-2(3)	6(3)	-4(3)
N(4)	22(3)	15(4)	26(3)	-2(2)	9(2)	-2(3)
O(1S')	16(3)	17(4)	16(4)	0(3)	-3(2)	1(3)
N(4')	15(3)	17(5)	21(3)	1(3)	8(3)	-3(3)

Table 5S. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **10**.

	x	y	z	U(eq)
H(9A)	7662	6476	7830	21
H(9B)	7669	4883	7669	21

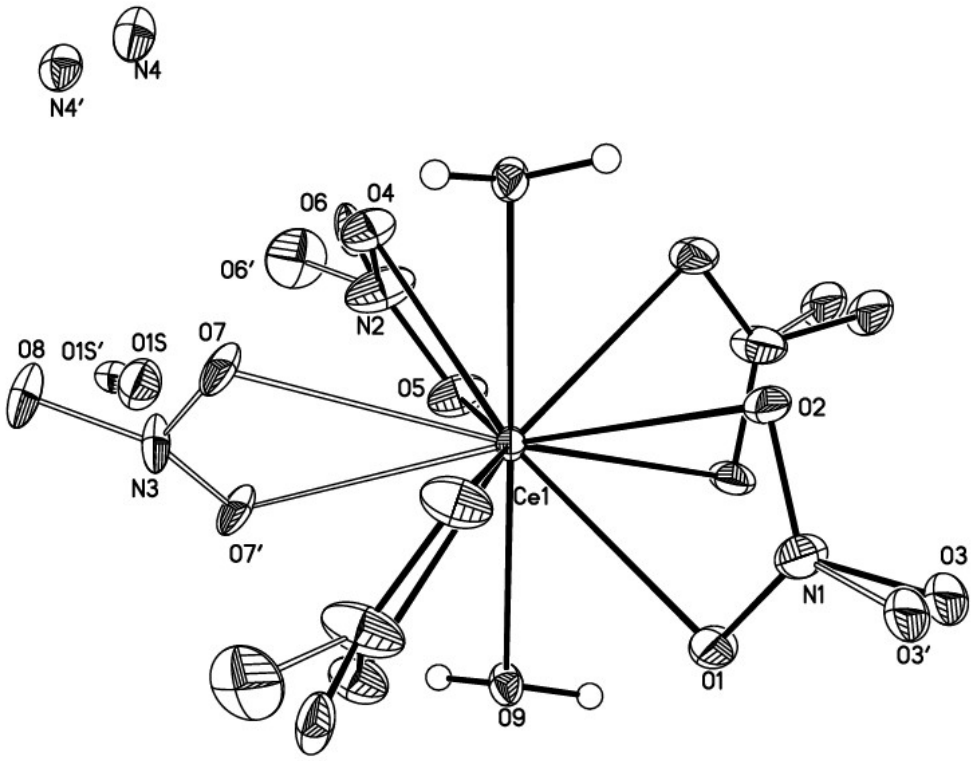
Table 6S. Torsion angles [°] for **10**.

Ce(1)-O(1)-N(1)-O(3)	-165.5(8)
Ce(1)-O(1)-N(1)-O(3')	161.6(6)
Ce(1)-O(1)-N(1)-O(2)	-6.8(5)
Ce(1)-O(2)-N(1)-O(3)	166.1(8)
Ce(1)-O(2)-N(1)-O(1)	6.6(5)
Ce(1)-O(2)-N(1)-O(3')	-161.9(6)
Ce(1)-O(5)-N(2)-O(6)	171.5(6)
Ce(1)-O(5)-N(2)-O(6')	-155.4(7)
Ce(1)-O(5)-N(2)-O(4)	9.2(5)
Ce(1)-O(4)-N(2)-O(6)	-170.8(7)
Ce(1)-O(4)-N(2)-O(5)	-9.1(5)
Ce(1)-O(4)-N(2)-O(6')	156.1(6)
O(7')-N(3)-O(7)-Ce(1)	-2(3)
O(8)-N(3)-O(7)-Ce(1)	-156.9(4)
O(7)-N(3)-O(7')-Ce(1)	2(3)
O(8)-N(3)-O(7')-Ce(1)	154.9(4)

Symmetry transformations used to generate equivalent atoms:

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

Projection view with 50% probability ellipsoids:



Compound 13

Table 7S. Crystal data and structure refinement for **13**.

Identification code	d12917/lt/x8/TB5-P122	
Empirical formula	C_{14} H_{19} N O_{12}	
Formula weight	393.30	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 5.5311(7) Å	α= 90°.
	b = 13.8941(17) Å	β= 90°.
	c = 23.168(3) Å	γ = 90°.
Volume	1780.4(4) $Å^3$	
Z	4	
Density (calculated)	1.467 Mg/m^3	
Absorption coefficient	0.131 mm^{-1}	
F(000)	824	
Crystal size	0.627 x 0.088 x 0.077 mm^3	
Theta range for data collection	1.709 to 27.567°.	
Index ranges	-5≤h≤7, -18≤k≤17, -26≤l≤30	
Reflections collected	22069	
Independent reflections	4099 [R(int) = 0.0605]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9420 and 0.8656	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4099 / 0 / 248	
Goodness-of-fit on F^2	1.016	
Final R indices [I>2sigma(I)]	R1 = 0.0416, wR2 = 0.0728	
R indices (all data)	R1 = 0.0715, wR2 = 0.0827	
Absolute structure parameter	0.4(7)	
Largest diff. peak and hole	0.201 and -0.252 $e.Å^{-3}$	

Table 8S. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **13**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	7567(3)	4658(1)	4269(1)	17(1)
O(2)	7638(3)	6280(1)	4363(1)	20(1)
O(3)	6410(5)	5992(2)	5281(1)	29(1)
O(4)	9349(4)	6989(2)	5098(1)	37(1)
O(5)	3772(3)	6421(1)	3540(1)	16(1)
O(6)	6617(4)	7394(1)	3157(1)	22(1)
O(7)	3930(3)	4808(1)	2752(1)	14(1)
O(8)	-147(3)	4733(2)	2788(1)	23(1)
O(9)	3729(3)	3068(1)	3407(1)	14(1)
O(10)	6630(3)	2142(1)	3008(1)	19(1)
O(11)	6460(3)	2123(1)	4344(1)	18(1)
O(12)	9908(4)	1299(2)	4469(1)	24(1)
N(1)	7789(5)	6423(2)	4977(1)	25(1)
C(1)	6144(5)	5492(2)	4207(1)	17(1)
C(2)	5459(5)	5640(2)	3578(1)	13(1)
C(3)	4123(5)	4749(2)	3371(1)	13(1)
C(4)	5454(5)	3824(2)	3514(1)	14(1)
C(5)	6196(5)	3803(2)	4149(1)	15(1)
C(6)	7895(5)	2993(2)	4311(1)	20(1)
C(7)	7733(5)	1306(2)	4435(1)	16(1)
C(8)	6105(5)	463(2)	4506(1)	21(1)
C(9)	4566(5)	7268(2)	3315(1)	16(1)
C(10)	2573(5)	7982(2)	3301(1)	21(1)
C(11)	1682(5)	4771(2)	2512(1)	15(1)
C(12)	1884(5)	4777(2)	1872(1)	17(1)
C(13)	4556(5)	2253(2)	3148(1)	15(1)
C(14)	2550(5)	1545(2)	3095(1)	18(1)

Table 9S. Bond lengths [Å] and angles [°] for **13**.

O(1)-C(1)	1.407(3)	C(9)-C(10)	1.484(4)
O(1)-C(5)	1.437(3)	C(10)-H(10A)	0.9800
O(2)-C(1)	1.419(3)	C(10)-H(10B)	0.9800
O(2)-N(1)	1.438(3)	C(10)-H(10C)	0.9800
O(3)-N(1)	1.199(3)	C(11)-C(12)	1.486(4)
O(4)-N(1)	1.200(3)	C(12)-H(12A)	0.9800
O(5)-C(9)	1.360(3)	C(12)-H(12B)	0.9800
O(5)-C(2)	1.433(3)	C(12)-H(12C)	0.9800
O(6)-C(9)	1.204(3)	C(13)-C(14)	1.487(4)
O(7)-C(11)	1.363(3)	C(14)-H(14A)	0.9800
O(7)-C(3)	1.439(3)	C(14)-H(14B)	0.9800
O(8)-C(11)	1.198(3)	C(14)-H(14C)	0.9800
O(9)-C(13)	1.360(3)		
O(9)-C(4)	1.441(3)	C(1)-O(1)-C(5)	111.42(19)
O(10)-C(13)	1.202(3)	C(1)-O(2)-N(1)	113.2(2)
O(11)-C(7)	1.353(3)	C(9)-O(5)-C(2)	117.9(2)
O(11)-C(6)	1.448(3)	C(11)-O(7)-C(3)	118.2(2)
O(12)-C(7)	1.206(3)	C(13)-O(9)-C(4)	117.4(2)
C(1)-C(2)	1.520(4)	C(7)-O(11)-C(6)	115.1(2)
C(1)-H(1)	1.0000	O(3)-N(1)-O(4)	130.3(3)
C(2)-C(3)	1.521(4)	O(3)-N(1)-O(2)	118.4(2)
C(2)-H(2)	1.0000	O(4)-N(1)-O(2)	111.3(3)
C(3)-C(4)	1.517(4)	O(1)-C(1)-O(2)	106.5(2)
C(3)-H(3)	1.0000	O(1)-C(1)-C(2)	110.4(2)
C(4)-C(5)	1.526(4)	O(2)-C(1)-C(2)	106.6(2)
C(4)-H(4)	1.0000	O(1)-C(1)-H(1)	111.1
C(5)-C(6)	1.514(4)	O(2)-C(1)-H(1)	111.1
C(5)-H(5)	1.0000	C(2)-C(1)-H(1)	111.1
C(6)-H(6A)	0.9900	O(5)-C(2)-C(1)	108.9(2)
C(6)-H(6B)	0.9900	O(5)-C(2)-C(3)	106.3(2)
C(7)-C(8)	1.486(4)	C(1)-C(2)-C(3)	108.2(2)
C(8)-H(8A)	0.9800	O(5)-C(2)-H(2)	111.1
C(8)-H(8B)	0.9800	C(1)-C(2)-H(2)	111.1
C(8)-H(8C)	0.9800	C(3)-C(2)-H(2)	111.1

O(7)-C(3)-C(4)	107.7(2)	C(7)-C(8)-H(8C)	109.5
O(7)-C(3)-C(2)	107.7(2)	H(8A)-C(8)-H(8C)	109.5
C(4)-C(3)-C(2)	112.6(2)	H(8B)-C(8)-H(8C)	109.5
O(7)-C(3)-H(3)	109.6	O(6)-C(9)-O(5)	123.1(3)
C(4)-C(3)-H(3)	109.6	O(6)-C(9)-C(10)	126.6(3)
C(2)-C(3)-H(3)	109.6	O(5)-C(9)-C(10)	110.3(2)
O(9)-C(4)-C(3)	104.9(2)	C(9)-C(10)-H(10A)	109.5
O(9)-C(4)-C(5)	109.3(2)	C(9)-C(10)-H(10B)	109.5
C(3)-C(4)-C(5)	111.0(2)	H(10A)-C(10)-H(10B)	109.5
O(9)-C(4)-H(4)	110.5	C(9)-C(10)-H(10C)	109.5
C(3)-C(4)-H(4)	110.5	H(10A)-C(10)-H(10C)	109.5
C(5)-C(4)-H(4)	110.5	H(10B)-C(10)-H(10C)	109.5
O(1)-C(5)-C(6)	103.8(2)	O(8)-C(11)-O(7)	123.6(3)
O(1)-C(5)-C(4)	108.2(2)	O(8)-C(11)-C(12)	126.6(3)
C(6)-C(5)-C(4)	114.9(2)	O(7)-C(11)-C(12)	109.8(2)
O(1)-C(5)-H(5)	109.9	C(11)-C(12)-H(12A)	109.5
C(6)-C(5)-H(5)	109.9	C(11)-C(12)-H(12B)	109.5
C(4)-C(5)-H(5)	109.9	H(12A)-C(12)-H(12B)	109.5
O(11)-C(6)-C(5)	107.0(2)	C(11)-C(12)-H(12C)	109.5
O(11)-C(6)-H(6A)	110.3	H(12A)-C(12)-H(12C)	109.5
C(5)-C(6)-H(6A)	110.3	H(12B)-C(12)-H(12C)	109.5
O(11)-C(6)-H(6B)	110.3	O(10)-C(13)-O(9)	123.1(2)
C(5)-C(6)-H(6B)	110.3	O(10)-C(13)-C(14)	127.2(3)
H(6A)-C(6)-H(6B)	108.6	O(9)-C(13)-C(14)	109.6(2)
O(12)-C(7)-O(11)	122.4(3)	C(13)-C(14)-H(14A)	109.5
O(12)-C(7)-C(8)	126.2(3)	C(13)-C(14)-H(14B)	109.5
O(11)-C(7)-C(8)	111.3(2)	H(14A)-C(14)-H(14B)	109.5
C(7)-C(8)-H(8A)	109.5	C(13)-C(14)-H(14C)	109.5
C(7)-C(8)-H(8B)	109.5	H(14A)-C(14)-H(14C)	109.5
H(8A)-C(8)-H(8B)	109.5	H(14B)-C(14)-H(14C)	109.5

Table 10S. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **13**. 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}
O(1)	20(1)	11(1)	20(1)	0(1)	-6(1)	-1(1)
O(2)	26(1)	15(1)	20(1)	-3(1)	-4(1)	-5(1)
O(3)	44(1)	23(1)	22(1)	-1(1)	-2(1)	-5(1)
O(4)	42(1)	30(1)	40(2)	-10(1)	-16(1)	-13(1)
O(5)	16(1)	10(1)	24(1)	2(1)	2(1)	1(1)
O(6)	18(1)	15(1)	33(1)	4(1)	0(1)	-1(1)
O(7)	13(1)	16(1)	14(1)	2(1)	-1(1)	0(1)
O(8)	13(1)	29(1)	27(1)	2(1)	1(1)	-1(1)
O(9)	12(1)	11(1)	18(1)	-2(1)	0(1)	-1(1)
O(10)	14(1)	17(1)	27(1)	-4(1)	1(1)	2(1)
O(11)	20(1)	12(1)	22(1)	2(1)	-2(1)	0(1)
O(12)	22(1)	21(1)	28(1)	5(1)	-3(1)	2(1)
N(1)	34(2)	16(1)	24(2)	-6(1)	-10(1)	2(1)
C(1)	19(2)	11(1)	21(2)	-1(1)	-1(1)	-3(1)
C(2)	14(1)	9(1)	18(2)	2(1)	0(1)	2(1)
C(3)	14(1)	14(1)	12(2)	1(1)	0(1)	0(1)
C(4)	13(1)	10(1)	19(2)	0(1)	-1(1)	-3(1)
C(5)	17(2)	12(1)	16(2)	-1(1)	-2(1)	-4(1)
C(6)	24(2)	13(1)	22(2)	3(1)	-3(1)	-5(1)
C(7)	23(2)	16(2)	10(2)	-1(1)	-2(1)	2(1)
C(8)	28(2)	13(2)	22(2)	1(1)	3(1)	1(1)
C(9)	19(2)	12(2)	16(2)	0(1)	-3(1)	-2(1)
C(10)	20(2)	14(1)	29(2)	-1(1)	-5(1)	3(1)
C(11)	16(1)	9(1)	21(2)	2(1)	-3(1)	-1(1)
C(12)	18(1)	15(1)	19(2)	1(1)	-2(1)	-1(1)
C(13)	18(2)	12(1)	15(2)	0(1)	-2(1)	2(1)
C(14)	15(1)	16(2)	24(2)	-3(1)	1(1)	-1(1)

Table 11S. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **13**.

	x	y	z	U(eq)
H(1)	4674	5460	4457	20
H(2)	6922	5767	3336	16
H(3)	2470	4732	3545	16
H(4)	6902	3747	3260	16
H(5)	4724	3783	4399	18
H(6A)	9179	2923	4016	23
H(6B)	8667	3127	4688	23
H(8A)	4693	538	4254	31
H(8B)	5573	421	4909	31
H(8C)	6975	-126	4401	31
H(10A)	2428	8289	3680	32
H(10B)	1053	7656	3206	32
H(10C)	2921	8472	3009	32
H(12A)	2699	4189	1743	26
H(12B)	2822	5340	1750	26
H(12C)	264	4808	1702	26
H(14A)	1195	1842	2888	27
H(14B)	2018	1348	3481	27
H(14C)	3115	980	2881	27

Table 12S. Torsion angles [°] for **13**.

C(1)-O(2)-N(1)-O(3)	-11.5(3)
C(1)-O(2)-N(1)-O(4)	168.9(2)
C(5)-O(1)-C(1)-O(2)	177.1(2)
C(5)-O(1)-C(1)-C(2)	-67.6(3)
N(1)-O(2)-C(1)-O(1)	-81.5(3)
N(1)-O(2)-C(1)-C(2)	160.6(2)
C(9)-O(5)-C(2)-C(1)	107.6(3)
C(9)-O(5)-C(2)-C(3)	-135.9(2)
O(1)-C(1)-C(2)-O(5)	172.9(2)
O(2)-C(1)-C(2)-O(5)	-71.9(3)
O(1)-C(1)-C(2)-C(3)	57.7(3)
O(2)-C(1)-C(2)-C(3)	172.9(2)
C(11)-O(7)-C(3)-C(4)	115.2(3)
C(11)-O(7)-C(3)-C(2)	-123.2(3)
O(5)-C(2)-C(3)-O(7)	74.9(3)
C(1)-C(2)-C(3)-O(7)	-168.2(2)
O(5)-C(2)-C(3)-C(4)	-166.6(2)
C(1)-C(2)-C(3)-C(4)	-49.7(3)
C(13)-O(9)-C(4)-C(3)	139.5(2)
C(13)-O(9)-C(4)-C(5)	-101.4(3)
O(7)-C(3)-C(4)-O(9)	-73.8(3)
C(2)-C(3)-C(4)-O(9)	167.7(2)
O(7)-C(3)-C(4)-C(5)	168.3(2)
C(2)-C(3)-C(4)-C(5)	49.8(3)
C(1)-O(1)-C(5)-C(6)	-172.9(2)
C(1)-O(1)-C(5)-C(4)	64.7(3)
O(9)-C(4)-C(5)-O(1)	-169.9(2)
C(3)-C(4)-C(5)-O(1)	-54.7(3)
O(9)-C(4)-C(5)-C(6)	74.6(3)
C(3)-C(4)-C(5)-C(6)	-170.1(2)
C(7)-O(11)-C(6)-C(5)	174.4(2)
O(1)-C(5)-C(6)-O(11)	165.6(2)
C(4)-C(5)-C(6)-O(11)	-76.4(3)
C(6)-O(11)-C(7)-O(12)	-2.2(4)

C(6)-O(11)-C(7)-C(8)	175.8(2)
C(2)-O(5)-C(9)-O(6)	-1.4(4)
C(2)-O(5)-C(9)-C(10)	179.1(2)
C(3)-O(7)-C(11)-O(8)	3.3(4)
C(3)-O(7)-C(11)-C(12)	-176.3(2)
C(4)-O(9)-C(13)-O(10)	0.0(4)
C(4)-O(9)-C(13)-C(14)	177.8(2)

Table 13S. Hydrogen bonds for **13** [Å and °].

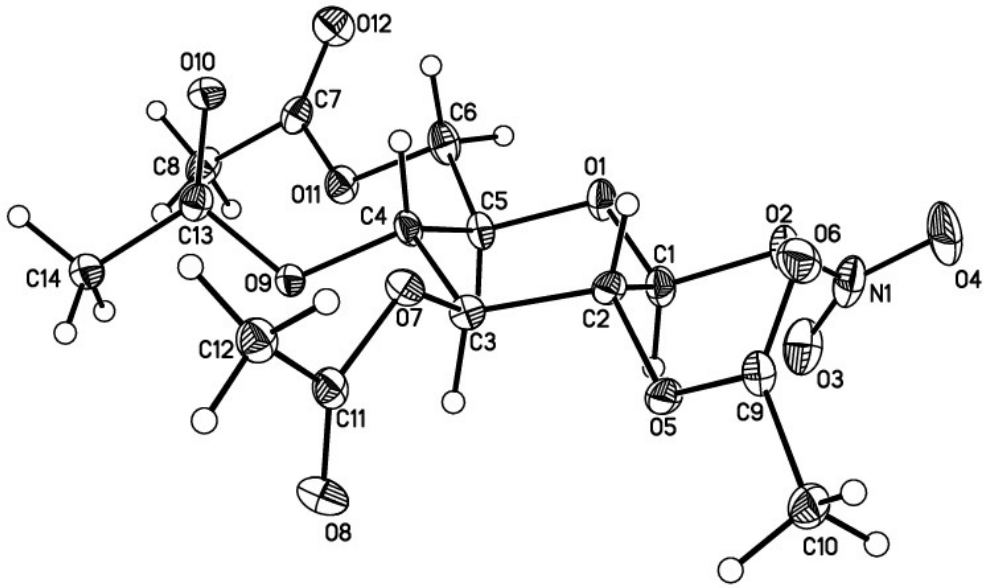
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...O(8)#1	1.00	2.51	3.293(3)	134.9
C(4)-H(4)...O(8)#1	1.00	2.40	3.217(3)	138.9
C(5)-H(5)...O(12)#2	1.00	2.63	3.284(4)	123.3
C(8)-H(8B)...O(1)#2	0.98	2.53	3.452(4)	156.4
C(10)-H(10B)...O(6)#3	0.98	2.48	3.410(3)	157.8
C(12)-H(12A)...O(6)#4	0.98	2.53	3.415(4)	149.5
C(12)-H(12B)...O(10)#5	0.98	2.58	3.398(4)	140.5
C(14)-H(14A)...O(10)#3	0.98	2.57	3.383(3)	140.0
C(14)-H(14B)...O(12)#3	0.98	2.57	3.519(4)	162.9

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+1,y-1/2,-z+1/2 #5 -x+1,y+1/2,-z+1/2

Projection view with 50% probability ellipsoids:



Compound 14

Table 14S. Crystal data and structure refinement for **14**.

Identification code	d14017_sq/lt/x8/Tb6-P33	
Empirical formula	C_{34} H_{27} N O_{12}	
Formula weight	641.56	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 14.9257(16) Å	α= 90°.
	b = 5.4551(6) Å	β= 95.990(7)°.
	c = 21.093(2) Å	γ = 90°.
Volume	1708.0(3) $Å^3$	
Z	2	
Density (calculated)	1.247 Mg/m^3	
Absorption coefficient	0.096 mm^{-1}	
F(000)	668	
Crystal size	0.578 x 0.109 x 0.075 mm^3	
Theta range for data collection	1.596 to 25.502°.	
Index ranges	-18≤h≤17, -6≤k≤6, -25≤l≤25	
Reflections collected	17263	
Independent reflections	6067 [R(int) = 0.0829]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9583 and 0.8124	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6067 / 471 / 497	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0789, wR2 = 0.1695	
R indices (all data)	R1 = 0.1668, wR2 = 0.2084	
Absolute structure parameter	0.5(10)	
Extinction coefficient	0.034(5)	
Largest diff. peak and hole	0.467 and -0.229 $e.Å^{-3}$	

Table 15S. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **14**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3140(3)	3962(10)	2193(3)	47(1)
O(2)	2177(4)	3326(12)	1322(3)	61(2)
O(3)	3341(5)	4394(16)	775(3)	89(2)
O(4)	2610(5)	1009(17)	567(4)	101(3)
O(5)	1097(3)	7264(11)	1669(2)	46(1)
O(6)	-133(4)	5212(12)	1926(3)	59(2)
O(7)	1165(3)	7500(9)	3031(2)	33(1)
O(8)	1400(4)	11503(10)	3229(3)	53(2)
O(9)	3047(3)	7720(10)	3604(2)	38(1)
O(10)	2264(5)	5816(16)	4297(3)	93(3)
O(11)	4988(3)	3920(11)	2772(3)	59(2)
O(12)	5196(7)	61(17)	3105(5)	79(3)
O(12')	5575(18)	1610(60)	3493(9)	79(3)
N(1)	2774(6)	2890(20)	846(4)	81(3)
C(1)	2486(5)	5113(17)	1774(4)	48(2)
C(2)	1666(5)	5784(15)	2109(3)	37(2)
C(3)	1946(4)	7288(16)	2691(3)	34(2)
C(4)	2705(5)	6062(15)	3110(3)	35(2)
C(5)	3480(5)	5482(15)	2717(4)	41(2)
C(6)	4179(5)	4017(17)	3110(4)	51(2)
C(7)	5510(6)	2020(20)	2892(5)	67(3)
C(8)	6370(20)	2400(80)	2610(30)	54(4)
C(9)	6387(12)	3430(40)	2022(10)	62(6)
C(10)	7211(12)	3550(40)	1709(10)	88(8)
C(11)	7982(14)	2560(50)	2042(12)	56(5)
C(12)	7970(20)	1320(70)	2595(17)	89(11)
C(13)	7185(14)	1260(50)	2883(13)	84(8)
C(8')	6410(20)	1850(90)	2660(30)	54(4)
C(9')	6746(12)	4150(40)	2575(11)	56(6)
C(10')	7679(12)	4350(40)	2424(10)	62(6)
C(11')	8122(18)	2130(60)	2392(17)	56(5)

C(12')	7652(16)	-180(50)	2479(12)	58(6)
C(13')	6862(15)	-60(50)	2624(11)	56(6)
C(14)	184(5)	6803(17)	1627(4)	44(2)
C(15)	-308(6)	8512(17)	1176(4)	50(2)
C(16)	-1236(6)	8080(20)	1026(4)	76(3)
C(17)	-1730(8)	9680(30)	607(5)	88(4)
C(18)	-1320(9)	11650(30)	353(5)	89(3)
C(19)	-400(8)	12010(20)	502(5)	81(3)
C(20)	100(7)	10505(19)	919(4)	64(3)
C(21)	977(5)	9678(14)	3300(4)	32(2)
C(22)	214(5)	9460(14)	3673(3)	34(2)
C(23)	-373(4)	7433(15)	3607(3)	34(2)
C(24)	-1072(5)	7241(16)	3983(4)	40(2)
C(25)	-1198(5)	9010(15)	4429(4)	39(2)
C(26)	-618(5)	11024(15)	4498(4)	42(2)
C(27)	90(5)	11253(14)	4124(4)	39(2)
C(28)	2789(5)	7350(20)	4197(4)	53(2)
C(29)	3080(17)	8750(50)	4745(12)	46(3)
C(30)	3060(18)	8120(50)	5381(13)	60(10)
C(31)	3380(20)	9740(60)	5859(11)	67(10)
C(32)	3730(30)	12000(50)	5700(13)	110(20)
C(33)	3750(30)	12640(40)	5063(14)	94(15)
C(34)	3420(20)	11010(50)	4586(11)	63(9)
C(29')	3278(8)	9200(20)	4635(5)	46(3)
C(30')	3015(8)	9380(30)	5246(6)	68(5)
C(31')	3451(8)	11010(40)	5681(5)	74(6)
C(32')	4150(8)	12460(30)	5505(5)	90(6)
C(33')	4413(10)	12280(20)	4894(5)	84(6)
C(34')	3977(10)	10640(20)	4459(4)	63(5)

Table 16S. Bond lengths [Å] and angles [°] for **14**.

O(1)-C(1)	1.396(10)	C(8)-C(13)	1.44(5)
O(1)-C(5)	1.433(9)	C(9)-C(10)	1.46(2)
O(2)-C(1)	1.407(9)	C(9)-H(9)	0.9500
O(2)-N(1)	1.430(9)	C(10)-C(11)	1.39(3)
O(3)-N(1)	1.197(11)	C(10)-H(10)	0.9500
O(4)-N(1)	1.197(11)	C(11)-C(12)	1.35(4)
O(5)-C(14)	1.380(9)	C(11)-H(11)	0.9500
O(5)-C(2)	1.438(9)	C(12)-C(13)	1.38(3)
O(6)-C(14)	1.200(9)	C(12)-H(12)	0.9500
O(7)-C(21)	1.359(8)	C(13)-H(13)	0.9500
O(7)-C(3)	1.435(7)	C(8')-C(13')	1.25(4)
O(8)-C(21)	1.197(8)	C(8')-C(9')	1.37(5)
O(9)-C(28)	1.361(10)	C(9')-C(10')	1.47(2)
O(9)-C(4)	1.433(9)	C(9')-H(9')	0.9500
O(10)-C(28)	1.182(11)	C(10')-C(11')	1.38(4)
O(11)-C(7)	1.306(11)	C(10')-H(10')	0.9500
O(11)-C(6)	1.466(8)	C(11')-C(12')	1.46(4)
O(12)-C(7)	1.268(12)	C(11')-H(11')	0.9500
O(12')-C(7)	1.281(15)	C(12')-C(13')	1.25(3)
C(1)-C(2)	1.520(10)	C(12')-H(12')	0.9500
C(1)-H(1)	1.0000	C(13')-H(13')	0.9500
C(2)-C(3)	1.500(10)	C(14)-C(15)	1.473(12)
C(2)-H(2)	1.0000	C(15)-C(20)	1.384(12)
C(3)-C(4)	1.517(10)	C(15)-C(16)	1.408(12)
C(3)-H(3)	1.0000	C(16)-C(17)	1.395(15)
C(4)-C(5)	1.525(10)	C(16)-H(16)	0.9500
C(4)-H(4)	1.0000	C(17)-C(18)	1.372(17)
C(5)-C(6)	1.494(11)	C(17)-H(17)	0.9500
C(5)-H(5)	1.0000	C(18)-C(19)	1.390(16)
C(6)-H(6A)	0.9900	C(18)-H(18)	0.9500
C(6)-H(6B)	0.9900	C(19)-C(20)	1.367(14)
C(7)-C(8')	1.475(15)	C(19)-H(19)	0.9500
C(7)-C(8)	1.479(14)	C(20)-H(20)	0.9500
C(8)-C(9)	1.36(5)	C(21)-C(22)	1.454(10)

C(22)-C(27)	1.390(10)	C(1)-O(1)-C(5)	113.4(6)
C(22)-C(23)	1.409(10)	C(1)-O(2)-N(1)	114.0(6)
C(23)-C(24)	1.379(9)	C(14)-O(5)-C(2)	116.8(6)
C(23)-H(23)	0.9500	C(21)-O(7)-C(3)	119.6(6)
C(24)-C(25)	1.375(11)	C(28)-O(9)-C(4)	117.5(6)
C(24)-H(24)	0.9500	C(7)-O(11)-C(6)	116.1(7)
C(25)-C(26)	1.398(11)	O(3)-N(1)-O(4)	129.5(9)
C(25)-H(25)	0.9500	O(3)-N(1)-O(2)	118.4(9)
C(26)-C(27)	1.390(10)	O(4)-N(1)-O(2)	112.1(8)
C(26)-H(26)	0.9500	O(1)-C(1)-O(2)	105.9(7)
C(27)-H(27)	0.9500	O(1)-C(1)-C(2)	111.0(6)
C(28)-C(29)	1.42(2)	O(2)-C(1)-C(2)	105.0(6)
C(28)-C(29')	1.503(13)	O(1)-C(1)-H(1)	111.5
C(29)-C(30)	1.3900	O(2)-C(1)-H(1)	111.5
C(29)-C(34)	1.3900	C(2)-C(1)-H(1)	111.5
C(30)-C(31)	1.3900	O(5)-C(2)-C(3)	108.5(6)
C(30)-H(30)	0.9500	O(5)-C(2)-C(1)	106.5(6)
C(31)-C(32)	1.3900	C(3)-C(2)-C(1)	110.0(6)
C(31)-H(31)	0.9500	O(5)-C(2)-H(2)	110.6
C(32)-C(33)	1.3900	C(3)-C(2)-H(2)	110.6
C(32)-H(32)	0.9500	C(1)-C(2)-H(2)	110.6
C(33)-C(34)	1.3900	O(7)-C(3)-C(2)	106.3(5)
C(33)-H(33)	0.9500	O(7)-C(3)-C(4)	109.9(5)
C(34)-H(34)	0.9500	C(2)-C(3)-C(4)	111.3(6)
C(29')-C(30')	1.3900	O(7)-C(3)-H(3)	109.7
C(29')-C(34')	1.3900	C(2)-C(3)-H(3)	109.7
C(30')-C(31')	1.3900	C(4)-C(3)-H(3)	109.7
C(30')-H(30')	0.9500	O(9)-C(4)-C(3)	109.5(6)
C(31')-C(32')	1.3900	O(9)-C(4)-C(5)	107.0(6)
C(31')-H(31')	0.9500	C(3)-C(4)-C(5)	109.7(6)
C(32')-C(33')	1.3900	O(9)-C(4)-H(4)	110.2
C(32')-H(32')	0.9500	C(3)-C(4)-H(4)	110.2
C(33')-C(34')	1.3900	C(5)-C(4)-H(4)	110.2
C(33')-H(33')	0.9500	O(1)-C(5)-C(6)	106.8(7)
C(34')-H(34')	0.9500	O(1)-C(5)-C(4)	108.1(6)
		C(6)-C(5)-C(4)	109.6(6)

O(1)-C(5)-H(5)	110.7	C(8')-C(9')-C(10')	118.0(19)
C(6)-C(5)-H(5)	110.7	C(8')-C(9')-H(9')	121.0
C(4)-C(5)-H(5)	110.7	C(10')-C(9')-H(9')	121.0
O(11)-C(6)-C(5)	108.2(6)	C(11')-C(10')-C(9')	114(2)
O(11)-C(6)-H(6A)	110.1	C(11')-C(10')-H(10')	122.8
C(5)-C(6)-H(6A)	110.1	C(9')-C(10')-H(10')	122.8
O(11)-C(6)-H(6B)	110.1	C(10')-C(11')-C(12')	121(2)
C(5)-C(6)-H(6B)	110.1	C(10')-C(11')-H(11')	119.7
H(6A)-C(6)-H(6B)	108.4	C(12')-C(11')-H(11')	119.7
O(12)-C(7)-O(11)	120.1(8)	C(13')-C(12')-C(11')	118(2)
O(12')-C(7)-O(11)	108.1(13)	C(13')-C(12')-H(12')	121.2
O(12')-C(7)-C(8')	110(3)	C(11')-C(12')-H(12')	121.2
O(11)-C(7)-C(8')	122.0(17)	C(12')-C(13')-C(8')	126(3)
O(12)-C(7)-C(8)	129.0(16)	C(12')-C(13')-H(13')	117.0
O(11)-C(7)-C(8)	109.4(15)	C(8')-C(13')-H(13')	117.0
C(9)-C(8)-C(13)	116.3(16)	O(6)-C(14)-O(5)	122.7(8)
C(9)-C(8)-C(7)	122(3)	O(6)-C(14)-C(15)	126.9(7)
C(13)-C(8)-C(7)	121(3)	O(5)-C(14)-C(15)	110.4(7)
C(8)-C(9)-C(10)	122.1(18)	C(20)-C(15)-C(16)	120.4(9)
C(8)-C(9)-H(9)	118.9	C(20)-C(15)-C(14)	122.7(8)
C(10)-C(9)-H(9)	118.9	C(16)-C(15)-C(14)	116.9(8)
C(11)-C(10)-C(9)	116.5(19)	C(17)-C(16)-C(15)	118.7(11)
C(11)-C(10)-H(10)	121.8	C(17)-C(16)-H(16)	120.7
C(9)-C(10)-H(10)	121.8	C(15)-C(16)-H(16)	120.7
C(12)-C(11)-C(10)	123(2)	C(18)-C(17)-C(16)	120.6(11)
C(12)-C(11)-H(11)	118.5	C(18)-C(17)-H(17)	119.7
C(10)-C(11)-H(11)	118.5	C(16)-C(17)-H(17)	119.7
C(11)-C(12)-C(13)	119(2)	C(17)-C(18)-C(19)	119.6(11)
C(11)-C(12)-H(12)	120.6	C(17)-C(18)-H(18)	120.2
C(13)-C(12)-H(12)	120.6	C(19)-C(18)-H(18)	120.2
C(12)-C(13)-C(8)	123(2)	C(20)-C(19)-C(18)	121.3(12)
C(12)-C(13)-H(13)	118.6	C(20)-C(19)-H(19)	119.4
C(8)-C(13)-H(13)	118.6	C(18)-C(19)-H(19)	119.4
C(13')-C(8')-C(9')	123.1(19)	C(19)-C(20)-C(15)	119.4(10)
C(13')-C(8')-C(7)	126(3)	C(19)-C(20)-H(20)	120.3
C(9')-C(8')-C(7)	110(3)	C(15)-C(20)-H(20)	120.3

O(8)-C(21)-O(7)	122.7(6)	C(29)-C(30)-H(30)	120.0
O(8)-C(21)-C(22)	126.1(7)	C(30)-C(31)-C(32)	120.0
O(7)-C(21)-C(22)	111.2(6)	C(30)-C(31)-H(31)	120.0
C(27)-C(22)-C(23)	119.6(7)	C(32)-C(31)-H(31)	120.0
C(27)-C(22)-C(21)	118.7(7)	C(33)-C(32)-C(31)	120.0
C(23)-C(22)-C(21)	121.7(7)	C(33)-C(32)-H(32)	120.0
C(24)-C(23)-C(22)	120.2(7)	C(31)-C(32)-H(32)	120.0
C(24)-C(23)-H(23)	119.9	C(34)-C(33)-C(32)	120.0
C(22)-C(23)-H(23)	119.9	C(34)-C(33)-H(33)	120.0
C(25)-C(24)-C(23)	120.4(8)	C(32)-C(33)-H(33)	120.0
C(25)-C(24)-H(24)	119.8	C(33)-C(34)-C(29)	120.0
C(23)-C(24)-H(24)	119.8	C(33)-C(34)-H(34)	120.0
C(24)-C(25)-C(26)	119.7(7)	C(29)-C(34)-H(34)	120.0
C(24)-C(25)-H(25)	120.1	C(30')-C(29')-C(34')	120.0
C(26)-C(25)-H(25)	120.1	C(30')-C(29')-C(28)	116.9(7)
C(27)-C(26)-C(25)	120.7(7)	C(34')-C(29')-C(28)	123.1(7)
C(27)-C(26)-H(26)	119.6	C(29')-C(30')-C(31')	120.0
C(25)-C(26)-H(26)	119.6	C(29')-C(30')-H(30')	120.0
C(26)-C(27)-C(22)	119.3(7)	C(31')-C(30')-H(30')	120.0
C(26)-C(27)-H(27)	120.4	C(32')-C(31')-C(30')	120.0
C(22)-C(27)-H(27)	120.4	C(32')-C(31')-H(31')	120.0
O(10)-C(28)-O(9)	121.7(9)	C(30')-C(31')-H(31')	120.0
O(10)-C(28)-C(29)	112.9(14)	C(33')-C(32')-C(31')	120.0
O(9)-C(28)-C(29)	125.4(14)	C(33')-C(32')-H(32')	120.0
O(10)-C(28)-C(29')	130.8(9)	C(31')-C(32')-H(32')	120.0
O(9)-C(28)-C(29')	107.5(8)	C(32')-C(33')-C(34')	120.0
C(30)-C(29)-C(34)	120.0	C(32')-C(33')-H(33')	120.0
C(30)-C(29)-C(28)	128.2(18)	C(34')-C(33')-H(33')	120.0
C(34)-C(29)-C(28)	111.8(18)	C(33')-C(34')-C(29')	120.0
C(31)-C(30)-C(29)	120.0	C(33')-C(34')-H(34')	120.0
C(31)-C(30)-H(30)	120.0	C(29')-C(34')-H(34')	120.0

Table 17S. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **14**. 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}
O(1)	32(3)	44(4)	67(4)	-9(3)	18(3)	0(3)
O(2)	39(3)	73(5)	75(4)	-32(3)	22(3)	-17(3)
O(3)	83(5)	114(6)	75(5)	-27(4)	36(4)	-32(5)
O(4)	88(6)	121(7)	98(6)	-64(6)	28(5)	-23(5)
O(5)	37(3)	55(4)	46(3)	2(3)	9(2)	-14(3)
O(6)	36(3)	67(5)	74(4)	14(3)	9(3)	-14(3)
O(7)	21(3)	27(3)	52(3)	-2(3)	14(2)	-2(2)
O(8)	51(4)	29(3)	82(4)	3(3)	22(3)	-12(3)
O(9)	31(3)	36(3)	48(3)	-5(3)	3(2)	-3(2)
O(10)	94(6)	130(7)	59(4)	-7(4)	28(4)	-61(5)
O(11)	30(3)	53(4)	99(5)	9(3)	28(3)	8(3)
O(12)	86(7)	64(7)	96(7)	23(5)	58(6)	33(5)
O(12')	86(7)	64(7)	96(7)	23(5)	58(6)	33(5)
N(1)	64(6)	112(8)	72(6)	-45(5)	28(5)	-29(5)
C(1)	35(5)	65(6)	47(5)	-14(4)	14(4)	-17(4)
C(2)	31(4)	39(5)	42(4)	-2(3)	9(3)	-8(3)
C(3)	23(4)	47(5)	36(4)	-6(4)	12(3)	-4(3)
C(4)	34(4)	32(4)	41(4)	2(3)	11(3)	0(3)
C(5)	28(4)	43(5)	54(5)	-2(4)	12(3)	-5(3)
C(6)	31(4)	49(6)	76(6)	11(5)	24(4)	2(4)
C(7)	49(5)	79(7)	79(6)	17(6)	32(5)	24(5)
C(8)	34(5)	48(13)	82(8)	1(9)	18(6)	11(5)
C(9)	37(9)	73(14)	79(12)	4(10)	25(9)	15(9)
C(10)	43(9)	130(20)	92(15)	50(14)	24(9)	23(11)
C(11)	17(6)	60(9)	92(17)	-8(10)	5(9)	-8(5)
C(12)	42(13)	90(20)	140(20)	49(18)	20(13)	36(15)
C(13)	47(11)	90(20)	112(18)	26(15)	17(11)	38(12)
C(8')	34(5)	48(13)	82(8)	1(9)	18(6)	11(5)
C(9')	30(8)	52(11)	88(17)	-18(11)	16(10)	-13(8)
C(10')	32(9)	68(10)	89(16)	-24(11)	25(10)	-17(8)
C(11')	17(6)	60(9)	92(17)	-8(10)	5(9)	-8(5)

C(12')	46(10)	48(11)	87(15)	-2(13)	35(11)	-5(8)
C(13')	49(11)	50(12)	75(17)	11(11)	32(11)	12(8)
C(14)	32(4)	54(6)	46(5)	-8(4)	5(4)	-10(4)
C(15)	47(5)	57(6)	47(5)	-5(4)	6(4)	2(4)
C(16)	47(5)	116(10)	66(6)	19(6)	6(5)	15(5)
C(17)	66(7)	127(10)	69(7)	12(7)	-4(6)	40(6)
C(18)	101(8)	94(9)	69(7)	8(6)	-3(6)	47(7)
C(19)	114(8)	70(8)	56(6)	1(5)	0(6)	27(6)
C(20)	79(7)	65(7)	47(5)	4(4)	-1(5)	-11(5)
C(21)	25(4)	21(4)	50(5)	0(3)	7(3)	1(3)
C(22)	29(4)	27(4)	46(5)	3(3)	5(3)	3(3)
C(23)	28(4)	33(4)	43(4)	-4(4)	8(3)	-2(3)
C(24)	22(4)	43(5)	56(5)	1(4)	10(3)	4(4)
C(25)	29(4)	40(5)	51(5)	2(4)	16(4)	9(3)
C(26)	35(5)	40(5)	50(5)	0(4)	6(4)	13(4)
C(27)	37(4)	32(5)	49(5)	-4(4)	5(4)	1(4)
C(28)	36(5)	72(6)	53(5)	-7(4)	12(4)	-2(4)
C(29)	12(6)	77(8)	50(6)	-11(6)	13(4)	12(5)
C(30)	26(17)	100(30)	54(10)	-7(12)	19(11)	-14(17)
C(31)	60(20)	70(20)	64(14)	-11(13)	8(16)	33(17)
C(32)	140(50)	90(20)	78(17)	-7(17)	-20(30)	-10(30)
C(33)	140(40)	53(17)	83(18)	9(13)	-40(20)	17(19)
C(34)	50(20)	72(14)	66(17)	4(12)	-9(16)	10(15)
C(29')	12(6)	77(8)	50(6)	-11(6)	13(4)	12(5)
C(30')	40(9)	117(16)	51(9)	-13(9)	17(7)	0(9)
C(31')	25(8)	129(19)	68(11)	-35(10)	3(7)	33(10)
C(32')	50(10)	146(17)	72(11)	-50(12)	-6(8)	0(10)
C(33')	36(10)	139(15)	78(9)	-46(10)	10(7)	-21(9)
C(34')	29(9)	101(11)	59(8)	-27(8)	5(7)	-16(7)

Table 18S. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **14**.

	x	y	z	U(eq)
H(1)	2736	6574	1567	58
H(2)	1340	4274	2225	44
H(3)	2141	8952	2562	41
H(4)	2483	4526	3300	42
H(5)	3746	7023	2562	49
H(6A)	4322	4792	3533	61
H(6B)	3953	2338	3175	61
H(9)	5846	4079	1809	74
H(10)	7222	4272	1300	105
H(11)	8542	2758	1871	67
H(12)	8493	497	2782	107
H(13)	7183	437	3279	101
H(9')	6385	5566	2611	67
H(10')	7957	5881	2353	74
H(11')	8737	2110	2314	67
H(12')	7937	-1711	2427	70
H(13')	6579	-1567	2712	68
H(16)	-1520	6733	1208	92
H(17)	-2355	9399	497	106
H(18)	-1663	12752	77	106
H(19)	-114	13335	310	97
H(20)	722	10824	1031	77
H(23)	-288	6196	3302	41
H(24)	-1468	5876	3934	48
H(25)	-1678	8864	4689	47
H(26)	-708	12251	4805	50
H(27)	486	12620	4175	47
H(30)	2824	6574	5490	72
H(31)	3369	9310	6294	80
H(32)	3949	13114	6026	126

H(33)	3984	14181	4954	113
H(34)	3439	11445	4151	76
H(30')	2537	8391	5366	82
H(31')	3271	11137	6099	88
H(32')	4448	13574	5802	108
H(33')	4891	13266	4773	101
H(34')	4157	10520	4041	76

Table 19S. Torsion angles [°] for **14**.

C(1)-O(2)-N(1)-O(3)	-17.4(13)
C(1)-O(2)-N(1)-O(4)	163.3(9)
C(5)-O(1)-C(1)-O(2)	-175.5(6)
C(5)-O(1)-C(1)-C(2)	-62.0(8)
N(1)-O(2)-C(1)-O(1)	-77.7(8)
N(1)-O(2)-C(1)-C(2)	164.7(7)
C(14)-O(5)-C(2)-C(3)	-103.5(7)
C(14)-O(5)-C(2)-C(1)	138.0(7)
O(1)-C(1)-C(2)-O(5)	171.7(6)
O(2)-C(1)-C(2)-O(5)	-74.3(8)
O(1)-C(1)-C(2)-C(3)	54.3(9)
O(2)-C(1)-C(2)-C(3)	168.3(7)
C(21)-O(7)-C(3)-C(2)	-138.9(7)
C(21)-O(7)-C(3)-C(4)	100.5(8)
O(5)-C(2)-C(3)-O(7)	72.9(7)
C(1)-C(2)-C(3)-O(7)	-170.9(7)
O(5)-C(2)-C(3)-C(4)	-167.4(5)
C(1)-C(2)-C(3)-C(4)	-51.2(8)
C(28)-O(9)-C(4)-C(3)	102.4(7)
C(28)-O(9)-C(4)-C(5)	-138.7(7)
O(7)-C(3)-C(4)-O(9)	-71.5(7)
C(2)-C(3)-C(4)-O(9)	170.9(6)
O(7)-C(3)-C(4)-C(5)	171.3(6)
C(2)-C(3)-C(4)-C(5)	53.8(8)
C(1)-O(1)-C(5)-C(6)	-178.9(6)

C(1)-O(1)-C(5)-C(4)	63.2(8)
O(9)-C(4)-C(5)-O(1)	-176.0(6)
C(3)-C(4)-C(5)-O(1)	-57.3(8)
O(9)-C(4)-C(5)-C(6)	67.9(8)
C(3)-C(4)-C(5)-C(6)	-173.4(7)
C(7)-O(11)-C(6)-C(5)	-153.3(8)
O(1)-C(5)-C(6)-O(11)	74.5(8)
C(4)-C(5)-C(6)-O(11)	-168.6(7)
C(6)-O(11)-C(7)-O(12)	22.5(15)
C(6)-O(11)-C(7)-O(12')	-42.4(18)
C(6)-O(11)-C(7)-C(8')	-171(4)
C(6)-O(11)-C(7)-C(8)	-170(3)
O(12)-C(7)-C(8)-C(9)	125(3)
O(11)-C(7)-C(8)-C(9)	-41(6)
O(12)-C(7)-C(8)-C(13)	-42(7)
O(11)-C(7)-C(8)-C(13)	152(4)
C(13)-C(8)-C(9)-C(10)	-5(6)
C(7)-C(8)-C(9)-C(10)	-173(3)
C(8)-C(9)-C(10)-C(11)	0(5)
C(9)-C(10)-C(11)-C(12)	6(4)
C(10)-C(11)-C(12)-C(13)	-8(5)
C(11)-C(12)-C(13)-C(8)	2(6)
C(9)-C(8)-C(13)-C(12)	4(7)
C(7)-C(8)-C(13)-C(12)	172(4)
O(12')-C(7)-C(8')-C(13')	70(8)
O(11)-C(7)-C(8')-C(13')	-162(5)
O(12')-C(7)-C(8')-C(9')	-102(4)
O(11)-C(7)-C(8')-C(9')	26(7)
C(13')-C(8')-C(9')-C(10')	0(9)
C(7)-C(8')-C(9')-C(10')	173(3)
C(8')-C(9')-C(10')-C(11')	-1(5)
C(9')-C(10')-C(11')-C(12')	3(4)
C(10')-C(11')-C(12')-C(13')	-5(4)
C(11')-C(12')-C(13')-C(8')	5(6)
C(9')-C(8')-C(13')-C(12')	-3(10)
C(7)-C(8')-C(13')-C(12')	-174(4)

C(2)-O(5)-C(14)-O(6)	-1.9(11)
C(2)-O(5)-C(14)-C(15)	178.1(6)
O(6)-C(14)-C(15)-C(20)	170.8(9)
O(5)-C(14)-C(15)-C(20)	-9.2(11)
O(6)-C(14)-C(15)-C(16)	-7.3(13)
O(5)-C(14)-C(15)-C(16)	172.8(8)
C(20)-C(15)-C(16)-C(17)	1.1(14)
C(14)-C(15)-C(16)-C(17)	179.2(9)
C(15)-C(16)-C(17)-C(18)	-0.9(16)
C(16)-C(17)-C(18)-C(19)	1.7(18)
C(17)-C(18)-C(19)-C(20)	-2.8(17)
C(18)-C(19)-C(20)-C(15)	2.9(15)
C(16)-C(15)-C(20)-C(19)	-2.1(14)
C(14)-C(15)-C(20)-C(19)	179.9(9)
C(3)-O(7)-C(21)-O(8)	5.5(10)
C(3)-O(7)-C(21)-C(22)	-174.4(6)
O(8)-C(21)-C(22)-C(27)	-18.5(11)
O(7)-C(21)-C(22)-C(27)	161.5(6)
O(8)-C(21)-C(22)-C(23)	164.4(8)
O(7)-C(21)-C(22)-C(23)	-15.7(10)
C(27)-C(22)-C(23)-C(24)	0.6(11)
C(21)-C(22)-C(23)-C(24)	177.8(7)
C(22)-C(23)-C(24)-C(25)	-0.5(11)
C(23)-C(24)-C(25)-C(26)	0.4(11)
C(24)-C(25)-C(26)-C(27)	-0.4(11)
C(25)-C(26)-C(27)-C(22)	0.5(11)
C(23)-C(22)-C(27)-C(26)	-0.6(11)
C(21)-C(22)-C(27)-C(26)	-177.8(7)
C(4)-O(9)-C(28)-O(10)	-4.0(13)
C(4)-O(9)-C(28)-C(29)	177.9(15)
C(4)-O(9)-C(28)-C(29')	176.3(7)
O(10)-C(28)-C(29)-C(30)	22(2)
O(9)-C(28)-C(29)-C(30)	-160.2(15)
O(10)-C(28)-C(29)-C(34)	-158.8(15)
O(9)-C(28)-C(29)-C(34)	20(2)
C(34)-C(29)-C(30)-C(31)	0.0

C(28)-C(29)-C(30)-C(31)	180(2)
C(29)-C(30)-C(31)-C(32)	0.0
C(30)-C(31)-C(32)-C(33)	0.0
C(31)-C(32)-C(33)-C(34)	0.0
C(32)-C(33)-C(34)-C(29)	0.0
C(30)-C(29)-C(34)-C(33)	0.0
C(28)-C(29)-C(34)-C(33)	-180(2)
O(10)-C(28)-C(29')-C(30')	-8.7(17)
O(9)-C(28)-C(29')-C(30')	171.0(8)
O(10)-C(28)-C(29')-C(34')	170.0(12)
O(9)-C(28)-C(29')-C(34')	-10.4(13)
C(34')-C(29')-C(30')-C(31')	0.0
C(28)-C(29')-C(30')-C(31')	178.7(11)
C(29')-C(30')-C(31')-C(32')	0.0
C(30')-C(31')-C(32')-C(33')	0.0
C(31')-C(32')-C(33')-C(34')	0.0
C(32')-C(33')-C(34')-C(29')	0.0
C(30')-C(29')-C(34')-C(33')	0.0
C(28)-C(29')-C(34')-C(33')	-178.6(12)

Table 20S. Hydrogen bonds for **14**_sq [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...O(8)#1	1.00	2.60	3.375(10)	134.7
C(4)-H(4)...O(8)#1	1.00	2.30	3.185(10)	146.4

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z

Projection view with 30% probability ellipsoids- disorder components omitted for clarity: