Supplementary Information

Peramivir analogues bearing hydrophilic side chains exhibit higher activities against H275Y mutant than wild-type influenza virus

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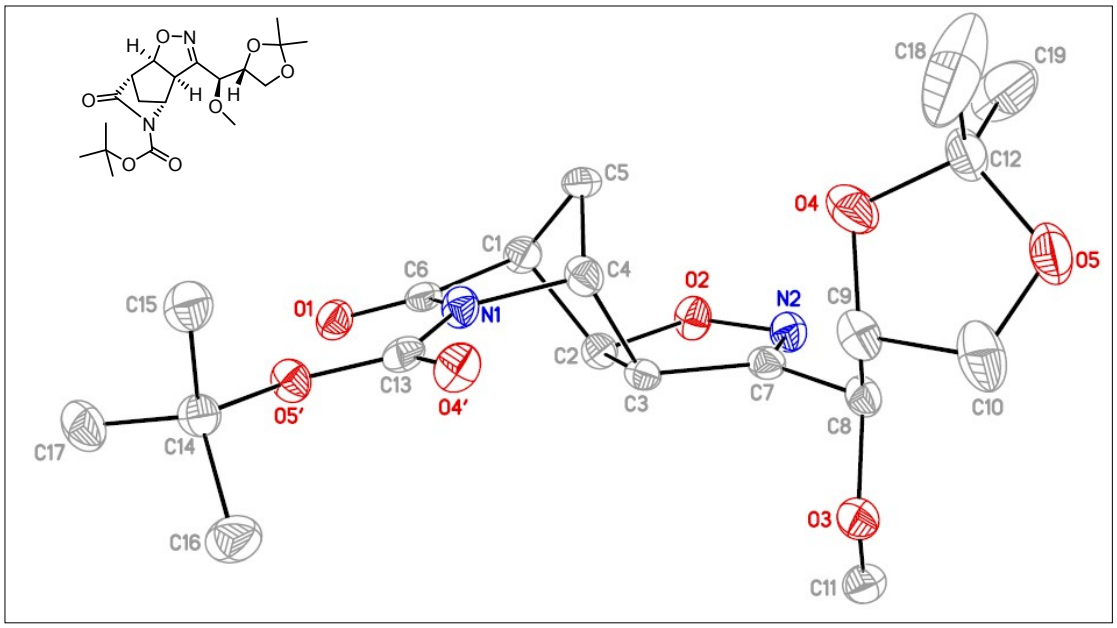


Fig. S1. ORTEP drawing of compound **22a** (IC17907, deposit CCDC 1570179); thermal ellipsoids drawn at the 50% probability level.

Table S1A. Crystal data and structure refinement for compound **22a** (ic17907).

Identification code	ic17907	
Empirical formula	C19 H28 N2 O7	
Formula weight	396.43	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Tetragonal	
Space group	P4(3)2(1)2	
Unit cell dimensions	a = 8.2526(2) Å	□= 90°.
	b = 8.2526(2) Å	□= 90°.
	c = 60.866(3) Å	□ = 90°.
Volume	4145.3(2) $Å^3$	
Z	8	
Density (calculated)	1.270 Mg/m^3	
Absorption coefficient	0.811 mm^{-1}	
F(000)	1696	
Crystal size	0.20 x 0.15 x 0.10 mm^3	
Theta range for data collection	2.90 to 67.98°.	
Index ranges	-9<=h<=6, -7<=k<=9, -72<=l<=72	
Reflections collected	14251	
Independent reflections	3755 [R(int) = 0.0403]	
Completeness to theta = 67.98°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.72594	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3755 / 6 / 253	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2sigma(I)]	R1 = 0.0728, wR2 = 0.1981	
R indices (all data)	R1 = 0.0798, wR2 = 0.2049	
Absolute structure parameter	0.0(4)	
Largest diff. peak and hole	1.070 and -0.289 $e.Å^{-3}$	

Table S1B. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for compound **22a** (ic17907). U (eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	7973(3)	1965(3)	1094(1)	40(1)
O(2)	6717(4)	463(3)	1805(1)	42(1)
O(3)	3949(4)	4757(4)	2012(1)	43(1)
O(4)	8219(4)	5336(4)	2110(1)	58(1)
O(5)	7174(5)	6368(7)	2426(1)	87(2)
O(4')	7392(4)	6706(4)	1353(1)	45(1)
O(5')	7544(3)	5272(3)	1037(1)	36(1)
N(1)	7931(4)	4024(4)	1362(1)	36(1)
N(2)	6317(4)	1484(4)	1985(1)	40(1)
C(1)	8291(5)	1410(5)	1489(1)	40(1)
C(2)	6625(5)	1393(5)	1601(1)	34(1)
C(3)	6358(4)	3170(4)	1675(1)	30(1)
C(4)	7989(5)	3961(5)	1604(1)	38(1)
C(5)	9213(5)	2588(6)	1637(1)	45(1)
C(6)	8066(4)	2439(5)	1283(1)	34(1)
C(7)	6115(4)	2935(5)	1918(1)	33(1)
C(8)	5529(5)	4211(5)	2074(1)	37(1)
C(9)	6575(6)	5731(5)	2072(1)	47(1)
C(10)	6113(8)	6878(7)	2260(1)	71(2)
C(11)	2762(5)	3523(6)	2012(1)	48(1)
C(12)	8649(7)	5892(11)	2323(1)	91(2)
C(13)	7590(4)	5466(4)	1252(1)	32(1)
C(14)	7493(5)	6720(5)	889(1)	37(1)
C(15)	8972(6)	7765(5)	936(1)	46(1)
C(16)	5943(6)	7644(6)	919(1)	58(1)
C(17)	7603(6)	5958(6)	664(1)	50(1)
C(18)	9816(13)	7213(18)	2305(2)	269(12)
C(19)	9295(10)	4390(20)	2445(1)	263(11)

Table S1C. Bond lengths [Å] and angles [°] for compound **22a** (ic17907).

O(1)-C(6)	1.217(4)
O(2)-N(2)	1.420(4)
O(2)-C(2)	1.463(4)
O(3)-C(11)	1.413(5)
O(3)-C(8)	1.431(5)
O(4)-C(9)	1.415(6)
O(4)-C(12)	1.418(6)
O(5)-C(10)	1.401(7)
O(5)-C(12)	1.424(8)
O(4')-C(13)	1.205(5)
O(5')-C(13)	1.322(4)
O(5')-C(14)	1.496(4)
N(1)-C(13)	1.392(5)
N(1)-C(6)	1.397(5)
N(1)-C(4)	1.477(4)
N(2)-C(7)	1.276(5)
C(1)-C(6)	1.526(5)
C(1)-C(5)	1.529(6)
C(1)-C(2)	1.534(5)
C(2)-C(3)	1.551(5)
C(3)-C(7)	1.504(4)
C(3)-C(4)	1.557(5)
C(4)-C(5)	1.532(6)
C(7)-C(8)	1.500(5)
C(8)-C(9)	1.523(6)
C(9)-C(10)	1.535(7)
C(12)-C(18)	1.458(11)
C(12)-C(19)	1.538(15)
C(14)-C(16)	1.499(6)
C(14)-C(17)	1.512(6)
C(14)-C(15)	1.522(6)

N(2)-O(2)-C(2)	109.4(3)
C(11)-O(3)-C(8)	113.9(3)
C(9)-O(4)-C(12)	108.5(4)
C(10)-O(5)-C(12)	107.5(4)
C(13)-O(5')-C(14)	120.1(3)
C(13)-N(1)-C(6)	130.7(3)
C(13)-N(1)-C(4)	120.9(3)
C(6)-N(1)-C(4)	107.9(3)
C(7)-N(2)-O(2)	109.9(3)
C(6)-C(1)-C(5)	101.1(3)
C(6)-C(1)-C(2)	105.1(3)
C(5)-C(1)-C(2)	100.9(3)
O(2)-C(2)-C(1)	109.6(3)
O(2)-C(2)-C(3)	104.8(3)
C(1)-C(2)-C(3)	104.3(3)
C(7)-C(3)-C(2)	100.6(3)
C(7)-C(3)-C(4)	116.3(3)
C(2)-C(3)-C(4)	101.1(3)
N(1)-C(4)-C(5)	100.3(3)
N(1)-C(4)-C(3)	105.3(3)
C(5)-C(4)-C(3)	102.9(3)
C(1)-C(5)-C(4)	93.7(3)

O(1)-C(6)-N(1)	128.3(3)
O(1)-C(6)-C(1)	127.3(4)
N(1)-C(6)-C(1)	104.4(3)
N(2)-C(7)-C(8)	119.8(3)
N(2)-C(7)-C(3)	114.7(3)
C(8)-C(7)-C(3)	125.2(3)
O(3)-C(8)-C(7)	110.3(3)
O(3)-C(8)-C(9)	104.7(3)
C(7)-C(8)-C(9)	112.8(3)
O(4)-C(9)-C(8)	110.6(4)
O(4)-C(9)-C(10)	104.8(4)
C(8)-C(9)-C(10)	111.0(4)
O(5)-C(10)-C(9)	101.4(5)
O(4)-C(12)-O(5)	106.1(4)
O(4)-C(12)-C(18)	109.8(5)
O(5)-C(12)-C(18)	113.0(8)
O(4)-C(12)-C(19)	105.5(8)
O(5)-C(12)-C(19)	107.8(5)
C(18)-C(12)-C(19)	114.1(9)
O(4')-C(13)-O(5')	127.2(3)
O(4')-C(13)-N(1)	120.6(3)
O(5')-C(13)-N(1)	112.1(3)
O(5')-C(14)-C(16)	111.0(3)
O(5')-C(14)-C(17)	102.2(3)
C(16)-C(14)-C(17)	111.8(4)
O(5')-C(14)-C(15)	108.4(3)
C(16)-C(14)-C(15)	111.9(4)
C(17)-C(14)-C(15)	111.0(4)

Symmetry transformations used to generate equivalent atoms:

Table S1D. Anisotropic displacement parameters ($Å^2 \times 10^3$) for compound **22a** (ic17907). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	41(2)	43(2)	38(1)	4(1)	7(1)	8(1)
O(2)	54(2)	34(1)	39(1)	10(1)	6(1)	4(1)
O(3)	44(2)	46(2)	39(1)	4(1)	-2(1)	6(1)
O(4)	56(2)	66(2)	51(2)	1(2)	-16(2)	-16(2)
O(5)	70(2)	156(4)	34(1)	-11(2)	5(2)	-45(3)
O(4')	46(2)	41(2)	47(1)	2(1)	8(1)	1(1)
O(5')	42(2)	30(1)	37(1)	8(1)	-1(1)	-1(1)
N(1)	39(2)	34(2)	34(1)	5(1)	3(1)	-5(1)
N(2)	43(2)	42(2)	35(2)	4(1)	1(1)	0(2)
C(1)	37(2)	42(2)	40(2)	11(2)	3(2)	13(2)
C(2)	35(2)	32(2)	35(2)	7(1)	0(2)	4(2)
C(3)	26(2)	32(2)	31(2)	3(1)	-4(1)	1(2)
C(4)	39(2)	40(2)	34(2)	6(2)	-3(2)	-8(2)
C(5)	23(2)	73(3)	39(2)	15(2)	-1(2)	0(2)
C(6)	21(2)	44(2)	37(2)	9(2)	3(1)	7(2)
C(7)	27(2)	39(2)	34(2)	8(2)	-2(1)	-4(2)
C(8)	42(2)	42(2)	28(2)	4(2)	-3(2)	3(2)
C(9)	58(3)	44(2)	38(2)	1(2)	-7(2)	-6(2)
C(10)	102(4)	62(3)	48(2)	-16(2)	-7(3)	-19(3)
C(11)	37(2)	60(3)	47(2)	6(2)	3(2)	2(2)
C(12)	55(3)	184(6)	33(2)	-10(3)	1(2)	-47(4)
C(13)	24(2)	30(2)	43(2)	5(2)	5(1)	-6(1)
C(14)	36(2)	33(2)	42(2)	11(2)	0(2)	-1(2)
C(15)	47(2)	42(2)	50(2)	12(2)	4(2)	-1(2)
C(16)	44(3)	58(3)	71(3)	23(2)	8(2)	11(2)
C(17)	60(3)	48(2)	43(2)	15(2)	-6(2)	2(2)
C(18)	199(11)	430(20)	173(9)	-220(13)	130(9)	-253(15)
C(19)	80(5)	650(30)	57(4)	119(9)	17(4)	132(11)

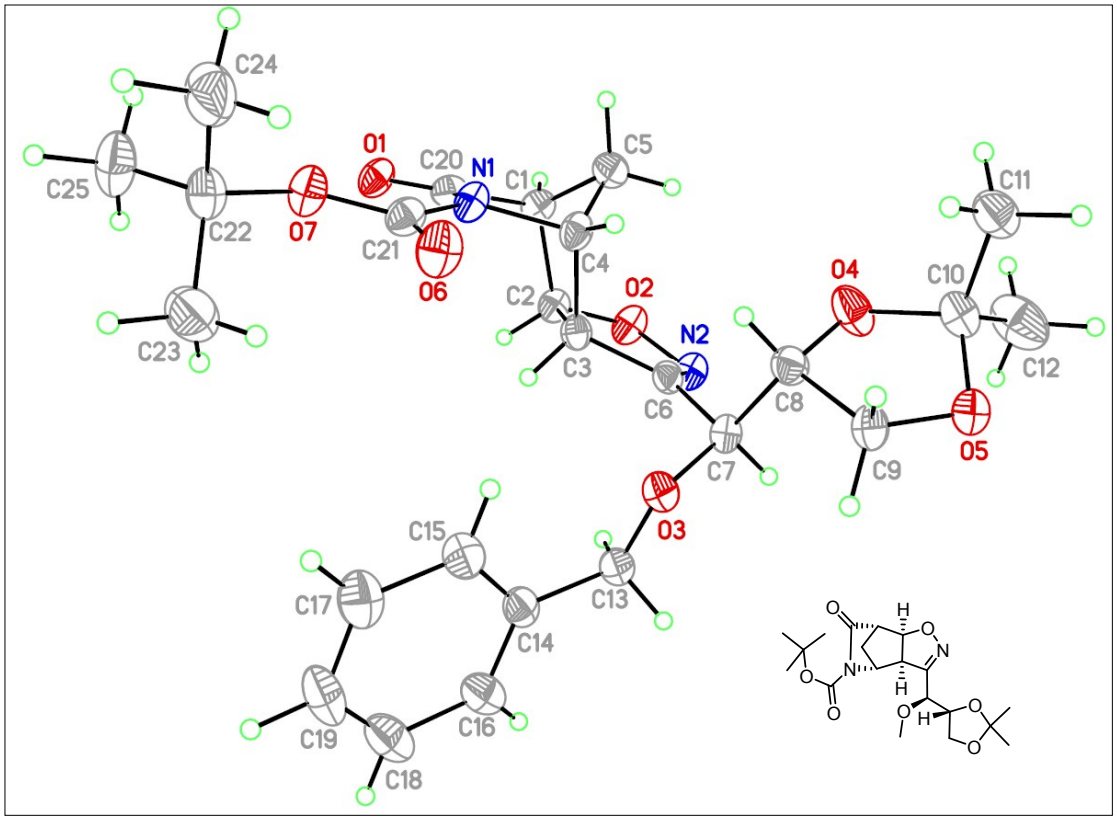


Fig. S2. ORTEP drawing of compound **22b** (IC18367, deposit CCDC 1570184); thermal ellipsoids drawn at the 50% probability level.

Table S2A. Crystal data and structure refinement for compound **22b** (ic18367).

Identification code	ic18367	
Empirical formula	C25 H32 N2 O7	
Formula weight	472.53	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 6.0765(2) Å	□= 89.902(3)°.
	b = 9.6451(4) Å	□= 75.421(3)°.
	c = 11.0698(4) Å	□ = 76.398(4)°.
Volume	609.14(4) $Å^3$	
Z	1	
Density (calculated)	1.288 Mg/m^3	
Absorption coefficient	0.779 mm^{-1}	
F(000)	252	
Crystal size	0.20 x 0.15 x 0.10 mm^3	
Theta range for data collection	4.13 to 67.97°.	
Index ranges	-7<=h<=7, -9<=k<=11, -13<=l<=13	
Reflections collected	9105	
Independent reflections	4153 [R(int) = 0.0271]	
Completeness to theta = 67.97°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.75261	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4153 / 3 / 307	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0342, wR2 = 0.0903	
R indices (all data)	R1 = 0.0361, wR2 = 0.0932	
Absolute structure parameter	-0.04(13)	
Largest diff. peak and hole	0.180 and -0.193 $e.Å^{-3}$	

Table S2B. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) of compound **22b** (ic18367). U (eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	6080(2)	13666(1)	1375(1)	31(1)
O(2)	4262(2)	9980(1)	-486(1)	32(1)
O(3)	6838(2)	6889(1)	2173(1)	26(1)
O(4)	10241(2)	6232(2)	-1025(1)	41(1)
O(5)	11292(2)	3956(1)	-504(1)	33(1)
O(6)	10157(2)	10206(2)	2813(1)	36(1)
O(7)	8620(2)	12596(1)	3060(1)	33(1)
N(1)	8490(2)	11375(2)	1371(1)	26(1)
N(2)	5018(3)	8485(2)	-345(2)	30(1)
C(1)	6478(3)	11722(2)	-163(2)	26(1)
C(2)	4842(3)	10778(2)	450(2)	25(1)
C(3)	6395(3)	9639(2)	1062(2)	23(1)
C(4)	8800(3)	10034(2)	634(2)	25(1)
C(5)	8801(3)	10606(2)	-655(2)	30(1)
C(6)	6191(3)	8297(2)	467(2)	23(1)
C(7)	7174(3)	6828(2)	858(2)	25(1)
C(8)	9823(3)	6320(2)	297(2)	27(1)
C(9)	10856(3)	4804(2)	626(2)	28(1)
C(10)	11757(3)	4871(2)	-1492(2)	32(1)
C(11)	14284(3)	4982(2)	-1835(2)	37(1)
C(12)	11071(5)	4336(4)	-2593(2)	57(1)
C(13)	4453(3)	7056(2)	2844(2)	28(1)
C(14)	4101(3)	7603(2)	4176(2)	28(1)
C(15)	5714(3)	8209(2)	4526(2)	34(1)
C(16)	2072(3)	7512(2)	5064(2)	36(1)
C(17)	5316(4)	8702(3)	5766(2)	41(1)
C(18)	1688(4)	8006(3)	6297(2)	44(1)
C(19)	3307(4)	8588(3)	6650(2)	43(1)
C(20)	6934(3)	12462(2)	939(2)	25(1)
C(21)	9170(3)	11313(2)	2492(2)	26(1)
C(22)	9299(3)	12804(2)	4236(2)	32(1)
C(23)	8249(4)	11915(3)	5236(2)	46(1)
C(24)	11956(4)	12472(3)	3954(2)	50(1)
C(25)	8194(5)	14388(3)	4562(2)	47(1)

Table S2C. Bond lengths [Å] and angles [°] for compound **22b** (ic18367).

O(1)-C(20)	1.202(2)
O(2)-N(2)	1.428(2)
O(2)-C(2)	1.450(2)
O(3)-C(7)	1.4174(19)
O(3)-C(13)	1.424(2)
O(4)-C(8)	1.420(2)
O(4)-C(10)	1.426(2)
O(5)-C(10)	1.418(2)
O(5)-C(9)	1.428(2)
O(6)-C(21)	1.197(2)
O(7)-C(21)	1.319(2)
O(7)-C(22)	1.488(2)
N(1)-C(21)	1.400(2)
N(1)-C(20)	1.408(2)
N(1)-C(4)	1.478(2)
N(2)-C(6)	1.269(2)
C(1)-C(20)	1.529(2)
C(1)-C(5)	1.533(2)
C(1)-C(2)	1.537(2)
C(2)-C(3)	1.546(2)
C(3)-C(6)	1.498(2)
C(3)-C(4)	1.555(2)
C(4)-C(5)	1.529(2)
C(6)-C(7)	1.510(2)
C(7)-C(8)	1.531(2)
C(8)-C(9)	1.532(2)
C(10)-C(12)	1.511(3)
C(10)-C(11)	1.516(3)
C(13)-C(14)	1.513(2)
C(14)-C(15)	1.384(3)
C(14)-C(16)	1.391(3)
C(15)-C(17)	1.396(3)
C(16)-C(18)	1.391(3)
C(17)-C(19)	1.385(3)
C(18)-C(19)	1.375(4)
C(22)-C(23)	1.506(3)
C(22)-C(24)	1.519(3)
C(22)-C(25)	1.521(3)
N(2)-O(2)-C(2)	109.52(12)
C(7)-O(3)-C(13)	113.07(12)
C(8)-O(4)-C(10)	108.31(14)
C(10)-O(5)-C(9)	106.05(14)
C(21)-O(7)-C(22)	120.39(14)
C(21)-N(1)-C(20)	130.27(15)
C(21)-N(1)-C(4)	119.35(14)
C(20)-N(1)-C(4)	107.88(14)
C(6)-N(2)-O(2)	109.27(14)
C(20)-C(1)-C(5)	101.85(14)
C(20)-C(1)-C(2)	104.35(13)
C(5)-C(1)-C(2)	101.39(14)
O(2)-C(2)-C(1)	111.15(14)
O(2)-C(2)-C(3)	104.83(13)
C(1)-C(2)-C(3)	103.78(13)

C(6)-C(3)-C(2)	100.58(13)
C(6)-C(3)-C(4)	116.68(13)
C(2)-C(3)-C(4)	101.63(13)
N(1)-C(4)-C(5)	100.41(14)
N(1)-C(4)-C(3)	104.65(13)
C(5)-C(4)-C(3)	103.39(13)
C(4)-C(5)-C(1)	93.40(13)
N(2)-C(6)-C(3)	115.06(15)
N(2)-C(6)-C(7)	122.16(16)
C(3)-C(6)-C(7)	122.68(14)
O(3)-C(7)-C(6)	108.91(13)
O(3)-C(7)-C(8)	105.95(12)
C(6)-C(7)-C(8)	111.95(14)
O(4)-C(8)-C(7)	107.88(13)
O(4)-C(8)-C(9)	104.74(14)
C(7)-C(8)-C(9)	113.21(14)
O(5)-C(9)-C(8)	103.85(13)
O(5)-C(10)-O(4)	104.84(14)
O(5)-C(10)-C(12)	108.11(19)
O(4)-C(10)-C(12)	109.36(18)
O(5)-C(10)-C(11)	112.40(16)
O(4)-C(10)-C(11)	109.79(17)
C(12)-C(10)-C(11)	112.06(17)
O(3)-C(13)-C(14)	109.70(14)
C(15)-C(14)-C(16)	119.41(17)
C(15)-C(14)-C(13)	121.94(16)
C(16)-C(14)-C(13)	118.64(17)
C(14)-C(15)-C(17)	120.00(18)
C(14)-C(16)-C(18)	120.2(2)
C(19)-C(17)-C(15)	120.3(2)
C(19)-C(18)-C(16)	120.4(2)
C(18)-C(19)-C(17)	119.73(19)
O(1)-C(20)-N(1)	127.87(16)
O(1)-C(20)-C(1)	128.33(16)
N(1)-C(20)-C(1)	103.71(14)
O(6)-C(21)-O(7)	128.14(16)
O(6)-C(21)-N(1)	120.96(17)
O(7)-C(21)-N(1)	110.89(15)
O(7)-C(22)-C(23)	110.79(16)
O(7)-C(22)-C(24)	108.99(15)
C(23)-C(22)-C(24)	112.59(19)
O(7)-C(22)-C(25)	101.15(15)
C(23)-C(22)-C(25)	110.97(18)
C(24)-C(22)-C(25)	111.8(2)

Symmetry transformations used to generate equivalent atoms:

Table S2D. Anisotropic displacement parameters ($Å^2 \times 10^3$) of compound **22b** (ic18367). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}\ U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	31(1)	19(1)	43(1)	0(1)	-13(1)	-3(1)
O(2)	31(1)	25(1)	43(1)	3(1)	-21(1)	-3(1)
O(3)	26(1)	28(1)	24(1)	0(1)	-6(1)	-3(1)
O(4)	39(1)	41(1)	28(1)	6(1)	-1(1)	9(1)
O(5)	36(1)	27(1)	34(1)	-5(1)	-4(1)	-6(1)
O(6)	42(1)	27(1)	39(1)	1(1)	-18(1)	0(1)
O(7)	43(1)	24(1)	34(1)	1(1)	-19(1)	-6(1)
N(1)	24(1)	21(1)	35(1)	-2(1)	-12(1)	-4(1)
N(2)	28(1)	26(1)	37(1)	0(1)	-13(1)	-5(1)
C(1)	27(1)	25(1)	28(1)	4(1)	-10(1)	-6(1)
C(2)	21(1)	23(1)	31(1)	0(1)	-9(1)	-2(1)
C(3)	22(1)	21(1)	24(1)	-1(1)	-6(1)	-1(1)
C(4)	23(1)	20(1)	33(1)	-3(1)	-9(1)	-1(1)
C(5)	26(1)	31(1)	31(1)	0(1)	-5(1)	-6(1)
C(6)	19(1)	24(1)	25(1)	-3(1)	-2(1)	-4(1)
C(7)	26(1)	22(1)	26(1)	-2(1)	-8(1)	-4(1)
C(8)	26(1)	24(1)	28(1)	3(1)	-5(1)	-3(1)
C(9)	26(1)	25(1)	29(1)	-2(1)	-6(1)	-1(1)
C(10)	28(1)	37(1)	28(1)	-1(1)	-5(1)	-2(1)
C(11)	31(1)	39(1)	35(1)	3(1)	-3(1)	-3(1)
C(12)	52(1)	90(2)	34(1)	-8(1)	-9(1)	-24(1)
C(13)	29(1)	28(1)	27(1)	-2(1)	-4(1)	-8(1)
C(14)	31(1)	22(1)	26(1)	1(1)	-6(1)	2(1)
C(15)	36(1)	34(1)	30(1)	0(1)	-7(1)	-8(1)
C(16)	33(1)	41(1)	31(1)	4(1)	-5(1)	-6(1)
C(17)	43(1)	41(1)	37(1)	-4(1)	-15(1)	-5(1)
C(18)	39(1)	53(1)	30(1)	3(1)	-1(1)	-2(1)
C(19)	47(1)	48(1)	25(1)	-8(1)	-8(1)	6(1)
C(20)	22(1)	24(1)	30(1)	5(1)	-7(1)	-6(1)
C(21)	23(1)	23(1)	31(1)	2(1)	-8(1)	-6(1)
C(22)	37(1)	32(1)	28(1)	-2(1)	-12(1)	-6(1)
C(23)	52(1)	45(1)	35(1)	3(1)	-6(1)	-10(1)
C(24)	39(1)	73(2)	40(1)	-15(1)	-12(1)	-16(1)
C(25)	73(2)	31(1)	41(1)	-4(1)	-26(1)	-8(1)

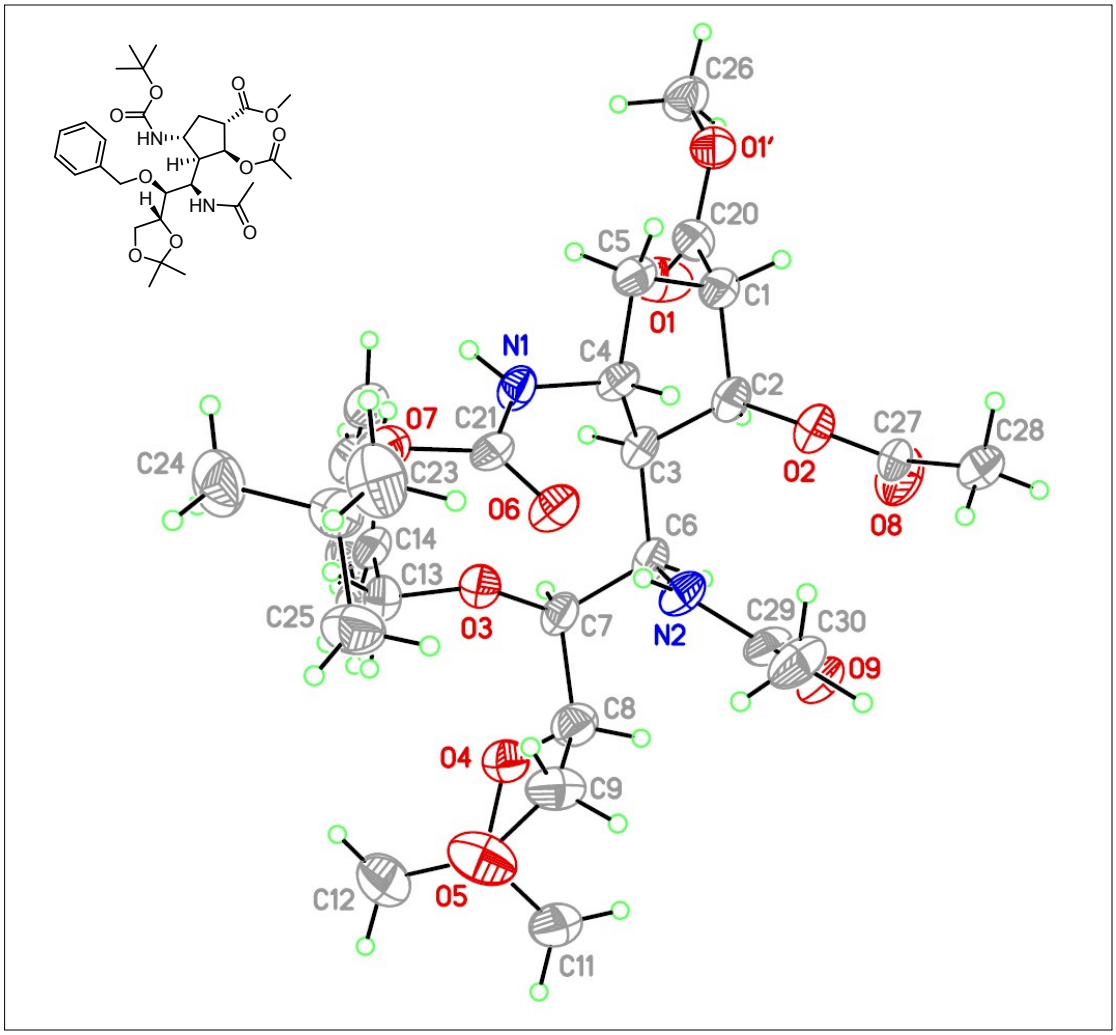


Fig. S3. ORTEP drawing of compound **23b** (IC18393, deposit CCDC 1570191); thermal ellipsoids drawn at the 50% probability level.

Table S3A. Crystal data and structure refinement for compound **23b** (ic18393).

Identification code	ic18393	
Empirical formula	C30 H44 N2 O10	
Formula weight	592.67	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.3732(4) Å	□= 90°.
	b = 16.8818(4) Å	□= 90°.
	c = 35.8766(11) Å	□ = 90°.
Volume	6282.6(3) $Å^3$	
Z	8	
Density (calculated)	1.253 Mg/m^3	
Absorption coefficient	0.778 mm^{-1}	
F(000)	2544	
Crystal size	0.30 x 0.15 x 0.10 mm^3	
Theta range for data collection	2.89 to 68.00°.	
Index ranges	-12<=h<=9, -20<=k<=16, -43<=l<=42	
Reflections collected	20260	
Independent reflections	10886 [R(int) = 0.0611]	
Completeness to theta = 68.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.40957	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10886 / 0 / 757	
Goodness-of-fit on F^2	1.175	
Final R indices [I>2sigma(I)]	R1 = 0.0798, wR2 = 0.2120	
R indices (all data)	R1 = 0.1223, wR2 = 0.2541	
Absolute structure parameter	-0.2(3)	
Largest diff. peak and hole	0.366 and -0.412 $e.Å^{-3}$	

Table S3B. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) of compound **23b** (ic18393). U (eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4408(5)	2889(3)	4840(2)	65(2)
O(2)	6710(4)	1140(2)	5321(1)	39(1)
O(3)	4363(4)	2217(2)	6429(1)	37(1)
O(4)	2111(4)	1050(2)	6544(1)	43(1)
O(5)	3106(5)	707(3)	7069(1)	64(1)
O(6)	7507(4)	2233(2)	6516(1)	40(1)
O(7)	6764(4)	3456(2)	6678(1)	38(1)
O(8)	5564(5)	306(3)	4964(1)	56(1)
O(9)	5904(4)	-258(2)	5970(1)	44(1)
O(1')	6218(4)	3307(2)	4575(1)	42(1)
N(1)	6613(5)	3076(3)	6091(1)	32(1)
N(2)	6118(5)	1030(3)	6152(1)	36(1)
C(1)	6427(6)	2465(3)	5093(2)	34(1)
C(2)	5735(6)	1769(3)	5289(2)	34(1)
C(3)	5440(6)	2046(3)	5683(2)	31(1)
C(4)	6669(6)	2541(3)	5772(2)	31(1)
C(5)	6871(6)	3022(3)	5415(2)	36(1)
C(6)	5019(6)	1356(3)	5944(2)	33(1)
C(7)	3909(6)	1584(3)	6198(2)	34(1)
C(8)	3411(6)	873(3)	6427(2)	41(1)
C(9)	4085(7)	679(4)	6791(2)	52(2)
C(10)	1916(7)	650(4)	6885(2)	47(2)
C(11)	1470(8)	-190(4)	6820(2)	58(2)
C(12)	932(8)	1110(5)	7113(2)	73(2)
C(13)	3384(6)	2718(3)	6597(2)	40(1)
C(14)	2451(6)	3073(3)	6318(2)	37(1)
C(15)	2898(7)	3615(3)	6053(2)	42(2)
C(16)	1158(6)	2877(4)	6325(2)	45(2)
C(17)	2083(7)	3957(4)	5801(2)	46(2)
C(18)	333(7)	3224(4)	6070(2)	51(2)
C(19)	777(7)	3760(4)	5807(2)	51(2)
C(20)	5560(6)	2895(4)	4825(2)	38(1)
C(21)	7006(6)	2870(3)	6431(2)	33(1)
C(22)	7108(6)	3379(4)	7072(2)	44(2)
C(23)	8567(7)	3300(5)	7110(2)	59(2)
C(24)	6645(8)	4162(4)	7232(2)	61(2)
C(25)	6388(7)	2698(4)	7246(2)	56(2)
C(26)	5454(7)	3783(3)	4320(2)	45(2)
C(27)	6534(6)	473(3)	5128(2)	35(1)
C(28)	7738(6)	-19(3)	5136(2)	44(2)
C(29)	6509(7)	272(3)	6134(2)	40(2)
C(30)	7775(6)	102(3)	6333(2)	49(2)
O(11)	4489(5)	7886(3)	4794(1)	60(1)
O(12)	6777(4)	6157(2)	5269(1)	35(1)
O(13)	4550(4)	7101(2)	6425(1)	36(1)
O(14)	2402(4)	5970(2)	6569(1)	41(1)
O(15)	3429(4)	4980(3)	6893(1)	52(1)
O(16)	7766(4)	7148(2)	6455(1)	39(1)
O(17)	6925(4)	8291(2)	6682(1)	41(1)

O(18)	5529(5)	5344(3)	4931(2)	58(1)
O(19)	6035(4)	4725(2)	5903(1)	41(1)
O(11')	6315(4)	8379(2)	4562(1)	40(1)
N(3)	6729(5)	8032(3)	6082(1)	33(1)
N(4)	6293(5)	5992(2)	6094(1)	33(1)
C(31)	6507(6)	7507(3)	5070(2)	32(1)
C(32)	5818(6)	6796(3)	5255(2)	34(1)
C(33)	5539(6)	7048(3)	5657(2)	30(1)
C(34)	6757(6)	7544(3)	5748(1)	31(1)
C(35)	6906(6)	8061(3)	5399(1)	34(1)
C(36)	5156(6)	6323(3)	5903(2)	31(1)
C(37)	4064(6)	6515(3)	6175(2)	30(1)
C(38)	3566(6)	5769(3)	6374(2)	38(1)
C(39)	4367(7)	5388(4)	6675(2)	46(2)
C(40)	2282(6)	5459(3)	6884(2)	42(2)
C(41)	1155(7)	4908(4)	6833(2)	55(2)
C(42)	2193(9)	5947(4)	7230(2)	67(2)
C(43)	3608(6)	7624(3)	6597(2)	40(2)
C(44)	2677(6)	8006(3)	6329(2)	37(1)
C(45)	3087(7)	8580(3)	6080(2)	44(2)
C(46)	1390(6)	7793(4)	6334(2)	44(2)
C(47)	2243(7)	8959(4)	5841(2)	47(2)
C(48)	535(7)	8168(4)	6093(2)	52(2)
C(49)	961(7)	8744(4)	5850(2)	53(2)
C(50)	5637(6)	7932(3)	4799(2)	36(1)
C(51)	7178(6)	7770(3)	6408(2)	36(1)
C(52)	7305(7)	8111(4)	7072(2)	49(2)
C(53)	8755(7)	8101(6)	7105(2)	74(3)
C(54)	6682(7)	7343(4)	7199(2)	52(2)
C(55)	6721(9)	8819(4)	7277(2)	70(2)
C(56)	5543(7)	8850(3)	4304(2)	43(2)
C(57)	6538(6)	5485(3)	5083(2)	35(1)
C(58)	7705(6)	4965(3)	5085(2)	42(1)
C(59)	6679(6)	5239(3)	6064(2)	35(1)
C(60)	7966(6)	5057(3)	6241(2)	44(2)

Table S3C. Bond lengths [Å] and angles [°] for compound **23b** (ic18393).

O(1)-C(20)	1.196(7)
O(2)-C(27)	1.334(6)
O(2)-C(2)	1.472(7)
O(3)-C(7)	1.431(6)
O(3)-C(13)	1.453(7)
O(4)-C(10)	1.410(7)
O(4)-C(8)	1.444(7)
O(5)-C(10)	1.404(8)
O(5)-C(9)	1.424(8)
O(6)-C(21)	1.232(7)
O(7)-C(21)	1.350(6)
O(7)-C(22)	1.464(7)
O(8)-C(27)	1.200(7)
O(9)-C(29)	1.242(7)
O(1')-C(20)	1.324(7)
O(1')-C(26)	1.454(7)
N(1)-C(21)	1.334(7)
N(1)-C(4)	1.457(6)
N(2)-C(29)	1.343(7)
N(2)-C(6)	1.471(7)
C(1)-C(20)	1.504(8)
C(1)-C(2)	1.546(8)
C(1)-C(5)	1.559(8)
C(2)-C(3)	1.521(8)
C(3)-C(6)	1.556(7)
C(3)-C(4)	1.558(8)
C(4)-C(5)	1.531(7)
C(6)-C(7)	1.519(8)
C(7)-C(8)	1.542(8)
C(8)-C(9)	1.517(8)
C(10)-C(11)	1.509(9)
C(10)-C(12)	1.522(10)
C(13)-C(14)	1.515(9)
C(14)-C(16)	1.382(9)
C(14)-C(15)	1.400(8)
C(15)-C(17)	1.364(9)
C(16)-C(18)	1.383(10)
C(17)-C(19)	1.396(10)
C(18)-C(19)	1.386(10)
C(22)-C(25)	1.507(9)
C(22)-C(24)	1.519(9)
C(22)-C(23)	1.526(9)
C(27)-C(28)	1.500(8)
C(29)-C(30)	1.521(9)
O(11)-C(50)	1.194(7)
O(12)-C(57)	1.341(6)
O(12)-C(32)	1.468(7)
O(13)-C(37)	1.425(6)
O(13)-C(43)	1.455(7)
O(14)-C(40)	1.428(7)
O(14)-C(38)	1.436(7)
O(15)-C(39)	1.427(7)
O(15)-C(40)	1.439(7)
O(16)-C(51)	1.225(7)

O(17)-C(51)	1.345(7)
O(17)-C(52)	1.483(7)
O(18)-C(57)	1.204(8)
O(19)-C(59)	1.240(7)
O(11')-C(50)	1.339(7)
O(11')-C(56)	1.458(7)
N(3)-C(51)	1.336(7)
N(3)-C(34)	1.454(6)
N(4)-C(59)	1.336(7)
N(4)-C(36)	1.474(7)
C(31)-C(50)	1.507(8)
C(31)-C(32)	1.548(8)
C(31)-C(35)	1.563(7)
C(32)-C(33)	1.529(7)
C(33)-C(34)	1.552(8)
C(33)-C(36)	1.562(7)
C(34)-C(35)	1.534(7)
C(36)-C(37)	1.530(8)
C(37)-C(38)	1.536(7)
C(38)-C(39)	1.506(8)
C(40)-C(42)	1.493(9)
C(40)-C(41)	1.505(9)
C(43)-C(44)	1.507(9)
C(44)-C(46)	1.382(9)
C(44)-C(45)	1.385(8)
C(45)-C(47)	1.381(9)
C(46)-C(48)	1.392(10)
C(47)-C(49)	1.378(10)
C(48)-C(49)	1.378(10)
C(52)-C(53)	1.509(10)
C(52)-C(54)	1.519(9)
C(52)-C(55)	1.530(10)
C(57)-C(58)	1.496(8)
C(59)-C(60)	1.509(9)

C(27)-O(2)-C(2)	118.3(5)
C(7)-O(3)-C(13)	116.4(4)
C(10)-O(4)-C(8)	106.7(5)
C(10)-O(5)-C(9)	107.1(5)
C(21)-O(7)-C(22)	121.4(5)
C(20)-O(1')-C(26)	115.9(5)
C(21)-N(1)-C(4)	123.0(4)
C(29)-N(2)-C(6)	124.5(5)
C(20)-C(1)-C(2)	112.3(5)
C(20)-C(1)-C(5)	111.0(4)
C(2)-C(1)-C(5)	105.0(4)
O(2)-C(2)-C(3)	106.7(4)
O(2)-C(2)-C(1)	105.4(5)
C(3)-C(2)-C(1)	106.4(4)
C(2)-C(3)-C(6)	112.6(4)
C(2)-C(3)-C(4)	101.0(5)
C(6)-C(3)-C(4)	120.5(5)
N(1)-C(4)-C(5)	109.5(4)
N(1)-C(4)-C(3)	117.4(5)
C(5)-C(4)-C(3)	103.0(4)
C(4)-C(5)-C(1)	105.1(4)

N(2)-C(6)-C(7)	112.1(5)
N(2)-C(6)-C(3)	111.6(5)
C(7)-C(6)-C(3)	112.6(4)
O(3)-C(7)-C(6)	106.7(5)
O(3)-C(7)-C(8)	112.6(5)
C(6)-C(7)-C(8)	112.1(5)
O(4)-C(8)-C(9)	102.9(5)
O(4)-C(8)-C(7)	107.9(5)
C(9)-C(8)-C(7)	118.1(5)
O(5)-C(9)-C(8)	105.5(5)
O(5)-C(10)-O(4)	104.4(5)
O(5)-C(10)-C(11)	114.0(6)
O(4)-C(10)-C(11)	111.2(5)
O(5)-C(10)-C(12)	107.6(6)
O(4)-C(10)-C(12)	108.5(6)
C(11)-C(10)-C(12)	110.8(6)
O(3)-C(13)-C(14)	113.8(5)
C(16)-C(14)-C(15)	119.3(6)
C(16)-C(14)-C(13)	120.9(6)
C(15)-C(14)-C(13)	119.7(6)
C(17)-C(15)-C(14)	121.4(6)
C(14)-C(16)-C(18)	119.2(6)
C(15)-C(17)-C(19)	119.4(6)
C(16)-C(18)-C(19)	121.4(7)
C(18)-C(19)-C(17)	119.3(7)
O(1)-C(20)-O(1')	123.4(6)
O(1)-C(20)-C(1)	124.4(6)
O(1')-C(20)-C(1)	112.2(5)
O(6)-C(21)-N(1)	125.6(5)
O(6)-C(21)-O(7)	123.9(5)
N(1)-C(21)-O(7)	110.5(5)
O(7)-C(22)-C(25)	110.4(5)
O(7)-C(22)-C(24)	102.2(5)
C(25)-C(22)-C(24)	110.5(6)
O(7)-C(22)-C(23)	109.7(5)
C(25)-C(22)-C(23)	112.8(6)
C(24)-C(22)-C(23)	110.8(6)
O(8)-C(27)-O(2)	124.6(5)
O(8)-C(27)-C(28)	125.2(5)
O(2)-C(27)-C(28)	110.2(5)
O(9)-C(29)-N(2)	123.8(6)
O(9)-C(29)-C(30)	121.5(5)
N(2)-C(29)-C(30)	114.8(5)
C(57)-O(12)-C(32)	118.6(5)
C(37)-O(13)-C(43)	116.7(4)
C(40)-O(14)-C(38)	108.4(4)
C(39)-O(15)-C(40)	106.2(5)
C(51)-O(17)-C(52)	120.2(5)
C(50)-O(11')-C(56)	115.0(5)
C(51)-N(3)-C(34)	121.8(5)
C(59)-N(4)-C(36)	124.3(5)
C(50)-C(31)-C(32)	111.7(5)
C(50)-C(31)-C(35)	111.2(4)
C(32)-C(31)-C(35)	105.2(4)
O(12)-C(32)-C(33)	107.5(4)
O(12)-C(32)-C(31)	105.8(5)

C(33)-C(32)-C(31)	106.0(4)
C(32)-C(33)-C(34)	101.3(5)
C(32)-C(33)-C(36)	111.4(4)
C(34)-C(33)-C(36)	120.7(5)
N(3)-C(34)-C(35)	110.6(4)
N(3)-C(34)-C(33)	117.7(5)
C(35)-C(34)-C(33)	102.5(4)
C(34)-C(35)-C(31)	104.5(4)
N(4)-C(36)-C(37)	112.1(4)
N(4)-C(36)-C(33)	110.9(5)
C(37)-C(36)-C(33)	112.6(4)
O(13)-C(37)-C(36)	106.6(4)
O(13)-C(37)-C(38)	113.4(4)
C(36)-C(37)-C(38)	111.8(4)
O(14)-C(38)-C(39)	102.5(5)
O(14)-C(38)-C(37)	108.4(4)
C(39)-C(38)-C(37)	119.8(5)
O(15)-C(39)-C(38)	102.9(5)
O(14)-C(40)-O(15)	106.6(5)
O(14)-C(40)-C(42)	109.2(5)
O(15)-C(40)-C(42)	110.1(6)
O(14)-C(40)-C(41)	110.2(5)
O(15)-C(40)-C(41)	107.3(5)
C(42)-C(40)-C(41)	113.2(6)
O(13)-C(43)-C(44)	114.8(5)
C(46)-C(44)-C(45)	119.2(6)
C(46)-C(44)-C(43)	119.9(5)
C(45)-C(44)-C(43)	120.9(6)
C(47)-C(45)-C(44)	121.9(6)
C(44)-C(46)-C(48)	119.2(6)
C(49)-C(47)-C(45)	118.4(6)
C(49)-C(48)-C(46)	120.6(7)
C(47)-C(49)-C(48)	120.7(7)
O(11)-C(50)-O(11')	123.4(6)
O(11)-C(50)-C(31)	125.2(6)
O(11')-C(50)-C(31)	111.4(5)
O(16)-C(51)-N(3)	125.2(5)
O(16)-C(51)-O(17)	123.9(5)
N(3)-C(51)-O(17)	110.8(5)
O(17)-C(52)-C(53)	110.0(6)
O(17)-C(52)-C(54)	110.2(5)
C(53)-C(52)-C(54)	113.0(7)
O(17)-C(52)-C(55)	100.9(5)
C(53)-C(52)-C(55)	111.4(7)
C(54)-C(52)-C(55)	110.6(6)
O(18)-C(57)-O(12)	123.7(5)
O(18)-C(57)-C(58)	126.2(5)
O(12)-C(57)-C(58)	110.1(5)
O(19)-C(59)-N(4)	122.8(6)
O(19)-C(59)-C(60)	122.0(5)
N(4)-C(59)-C(60)	115.1(5)

Symmetry transformations used to generate equivalent atoms:

Table S3D. Anisotropic displacement parameters ($Å^2 \times 10^3$) of compound **23b** (ic18393). The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	38(3)	76(3)	80(4)	38(3)	1(3)	4(3)
O(2)	46(2)	27(2)	45(2)	-4(2)	-3(2)	5(2)
O(3)	39(2)	33(2)	40(2)	-2(2)	6(2)	0(2)
O(4)	44(2)	39(2)	45(2)	4(2)	4(2)	-3(2)
O(5)	55(3)	91(4)	47(3)	12(3)	-3(2)	-13(3)
O(6)	49(3)	27(2)	43(2)	2(2)	-7(2)	-2(2)
O(7)	55(3)	30(2)	30(2)	0(2)	0(2)	-2(2)
O(8)	55(3)	43(2)	72(3)	-18(2)	-10(3)	-5(3)
O(9)	54(3)	22(2)	55(3)	-1(2)	-2(2)	-3(2)
O(1')	53(3)	37(2)	35(2)	7(2)	3(2)	4(2)
N(1)	40(3)	23(2)	33(2)	-5(2)	-4(2)	0(2)
N(2)	41(3)	23(2)	43(3)	-2(2)	-8(2)	-7(2)
C(1)	39(3)	29(3)	34(3)	-2(2)	1(3)	-2(3)
C(2)	37(3)	26(3)	40(3)	0(2)	-5(3)	7(3)
C(3)	35(3)	22(2)	37(3)	-2(2)	-2(3)	2(3)
C(4)	38(3)	21(2)	36(3)	1(2)	-3(3)	-3(3)
C(5)	43(3)	27(3)	37(3)	3(2)	1(3)	-2(3)
C(6)	41(3)	23(2)	35(3)	-4(2)	-8(3)	7(3)
C(7)	43(3)	22(2)	35(3)	-4(2)	-4(3)	1(3)
C(8)	47(4)	34(3)	43(3)	1(3)	-1(3)	-5(3)
C(9)	54(4)	51(4)	53(4)	18(3)	2(3)	-3(4)
C(10)	57(4)	48(3)	37(3)	3(3)	1(3)	-3(4)
C(11)	78(5)	42(3)	54(4)	6(3)	9(4)	-10(4)
C(12)	79(6)	70(5)	69(5)	-3(4)	35(5)	-8(5)
C(13)	48(4)	32(3)	40(3)	-8(3)	9(3)	0(3)
C(14)	48(4)	23(2)	40(3)	-4(2)	1(3)	-1(3)
C(15)	42(4)	30(3)	55(4)	-5(3)	3(3)	-8(3)
C(16)	46(4)	34(3)	54(4)	-8(3)	9(3)	-12(3)
C(17)	54(4)	34(3)	50(4)	1(3)	0(3)	1(3)
C(18)	49(4)	44(4)	60(4)	-11(3)	-1(4)	-4(3)
C(19)	57(4)	39(3)	57(4)	-4(3)	-6(4)	-1(4)
C(20)	45(4)	38(3)	31(3)	0(3)	4(3)	0(3)
C(21)	40(3)	21(2)	39(3)	-1(2)	3(3)	-9(3)
C(22)	45(4)	49(3)	36(3)	-2(3)	0(3)	-12(3)
C(23)	51(4)	78(5)	49(4)	-15(4)	-15(3)	1(4)
C(24)	79(5)	66(4)	37(3)	-14(3)	-5(4)	2(5)
C(25)	66(5)	61(4)	41(3)	12(3)	-1(3)	-8(4)
C(26)	64(4)	34(3)	38(3)	6(3)	-4(3)	5(3)
C(27)	40(4)	23(3)	41(3)	1(2)	7(3)	10(3)
C(28)	51(4)	28(3)	54(4)	-1(3)	6(3)	-6(3)
C(29)	51(4)	24(2)	44(3)	5(3)	3(3)	-8(3)
C(30)	44(4)	30(3)	74(4)	11(3)	-9(4)	4(3)
O(11)	41(3)	73(3)	66(3)	28(3)	-3(2)	2(3)
O(12)	40(2)	27(2)	39(2)	-4(2)	-3(2)	8(2)
O(13)	41(2)	27(2)	39(2)	-6(2)	4(2)	2(2)
O(14)	42(2)	35(2)	47(2)	6(2)	8(2)	-1(2)
O(15)	47(3)	53(3)	56(3)	18(2)	12(2)	-3(3)
O(16)	49(3)	30(2)	38(2)	4(2)	-6(2)	-2(2)
O(17)	55(3)	34(2)	35(2)	-6(2)	-1(2)	-9(2)

O(18)	52(3)	46(3)	75(3)	-20(3)	-13(3)	-2(3)
O(19)	54(3)	20(2)	50(2)	-1(2)	-2(2)	2(2)
O(11')	46(2)	38(2)	37(2)	8(2)	3(2)	-2(2)
N(3)	41(3)	24(2)	33(2)	-5(2)	-2(2)	-3(2)
N(4)	38(3)	22(2)	38(3)	1(2)	-3(2)	-8(2)
C(31)	37(3)	28(2)	31(3)	0(2)	0(3)	-2(3)
C(32)	38(3)	30(3)	34(3)	0(2)	-1(3)	8(3)
C(33)	33(3)	21(2)	35(3)	1(2)	-3(2)	2(3)
C(34)	37(3)	20(2)	35(3)	-1(2)	0(3)	-1(2)
C(35)	44(3)	27(2)	31(3)	1(2)	6(3)	0(3)
C(36)	37(3)	21(2)	33(3)	-1(2)	-2(2)	4(3)
C(37)	36(3)	22(2)	31(3)	-1(2)	-4(2)	3(3)
C(38)	42(4)	31(3)	39(3)	4(3)	5(3)	-5(3)
C(39)	43(4)	48(3)	48(4)	14(3)	4(3)	-6(3)
C(40)	46(4)	37(3)	43(3)	5(3)	8(3)	7(3)
C(41)	55(4)	36(3)	75(5)	6(3)	3(4)	-18(4)
C(42)	100(6)	49(4)	51(4)	-2(3)	18(4)	-10(5)
C(43)	53(4)	30(3)	35(3)	-3(2)	13(3)	0(3)
C(44)	51(4)	19(2)	42(3)	-1(2)	3(3)	5(3)
C(45)	51(4)	34(3)	48(3)	-2(3)	8(3)	-3(3)
C(46)	45(4)	32(3)	56(4)	-2(3)	10(3)	-7(3)
C(47)	54(4)	37(3)	51(4)	2(3)	2(3)	-9(3)
C(48)	42(4)	39(3)	76(5)	-10(4)	1(4)	-3(3)
C(49)	58(5)	40(3)	61(4)	-1(3)	-6(4)	1(4)
C(50)	45(4)	34(3)	30(3)	3(2)	2(3)	-1(3)
C(51)	40(3)	30(3)	36(3)	-1(3)	4(3)	-12(3)
C(52)	52(4)	62(4)	33(3)	-6(3)	3(3)	-9(4)
C(53)	60(5)	116(7)	44(4)	-5(5)	-5(4)	-12(5)
C(54)	56(4)	66(4)	35(3)	10(3)	-1(3)	-7(4)
C(55)	100(6)	70(5)	40(4)	-17(4)	8(4)	-19(5)
C(56)	59(4)	35(3)	35(3)	9(3)	-4(3)	9(3)
C(57)	47(4)	22(2)	36(3)	-1(2)	12(3)	7(3)
C(58)	47(4)	29(3)	49(3)	1(3)	5(3)	-6(3)
C(59)	43(4)	27(3)	36(3)	5(2)	2(3)	-7(3)
C(60)	40(4)	29(3)	63(4)	9(3)	-2(3)	4(3)

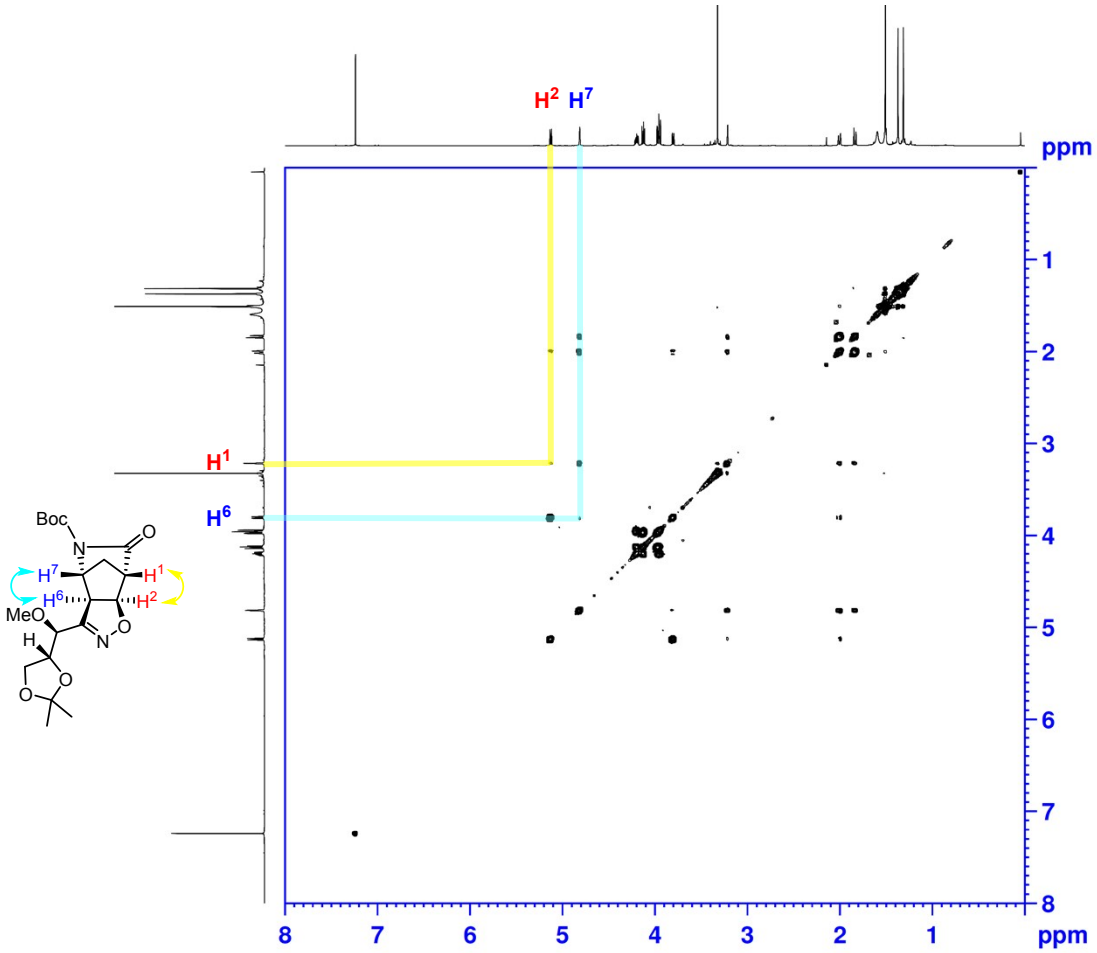


Fig. S4. ^{1}H–^{1}H COSY spectrum of isoxazoline **22a**.

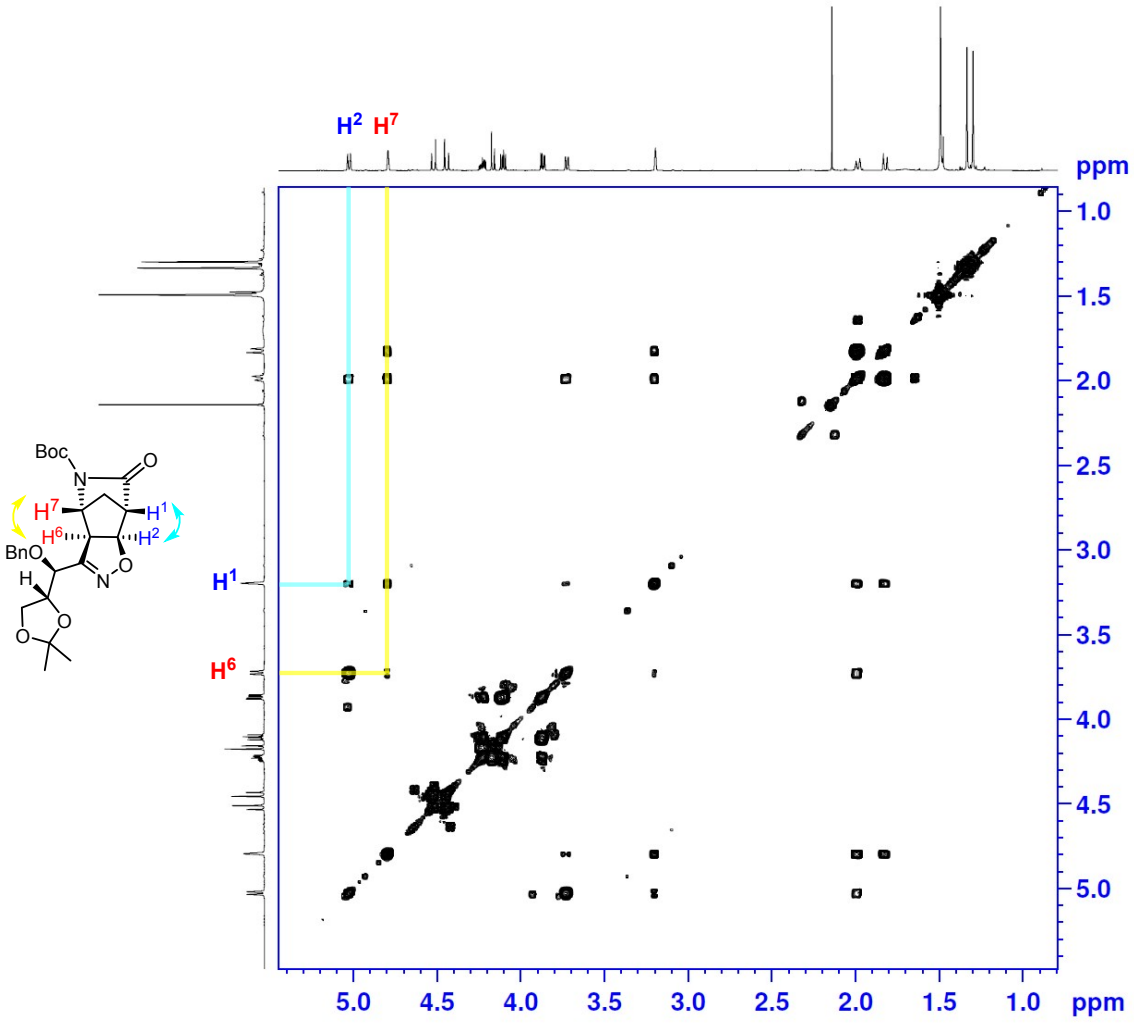
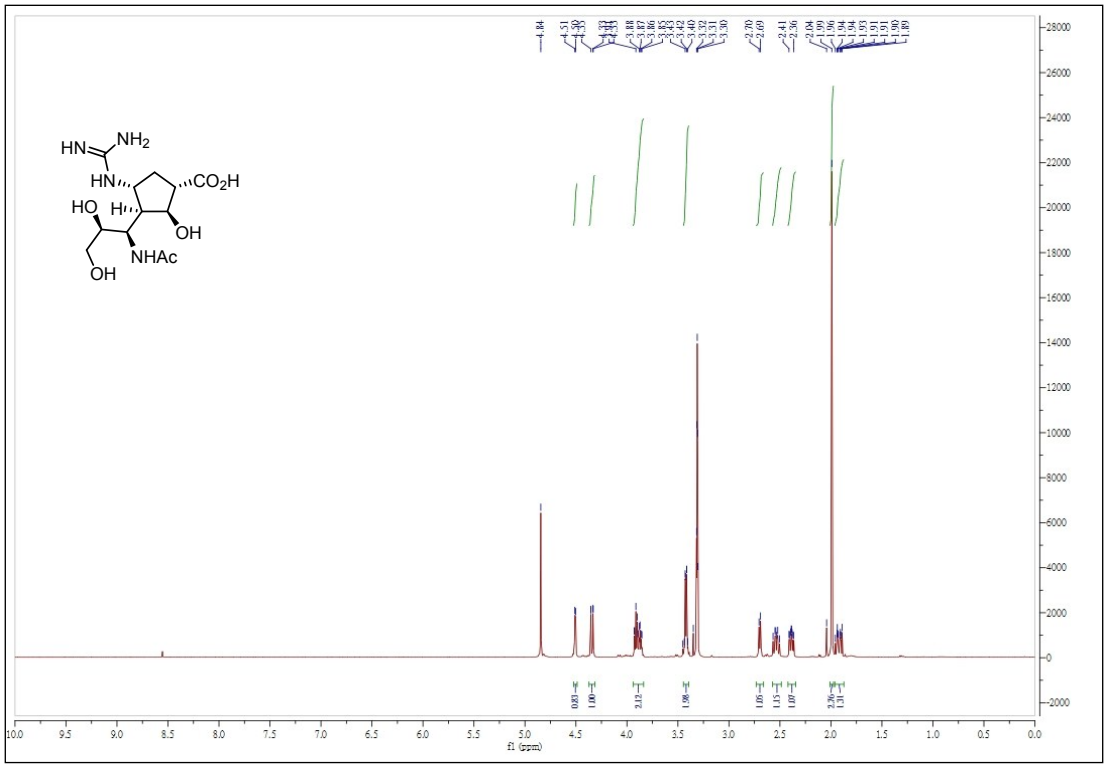
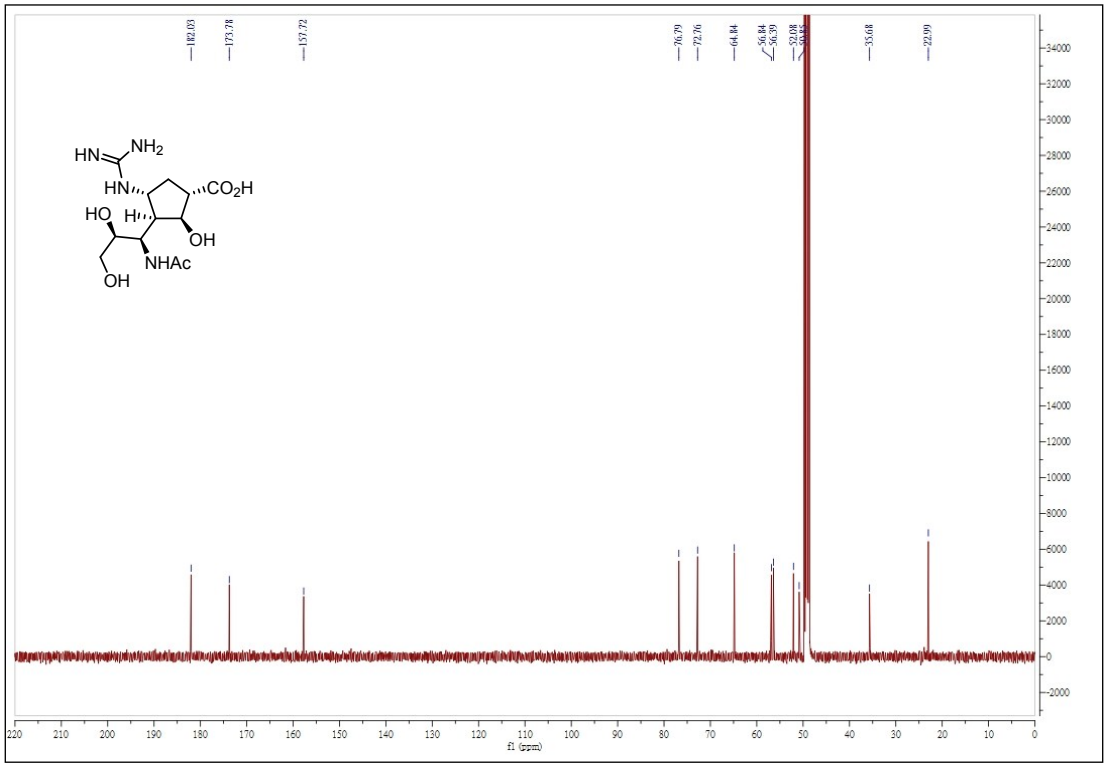


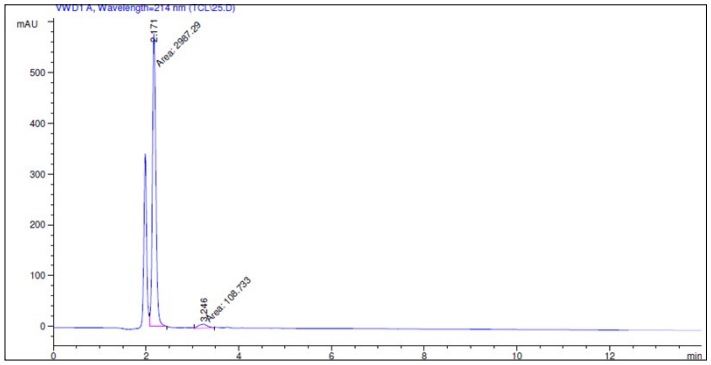
Fig. S5. ^{1}H–^{1}H COSY spectrum referring to isoxazoline **22b**.



^{1}H NMR spectrum of compound **5** (400 MHz, CD_3OD)

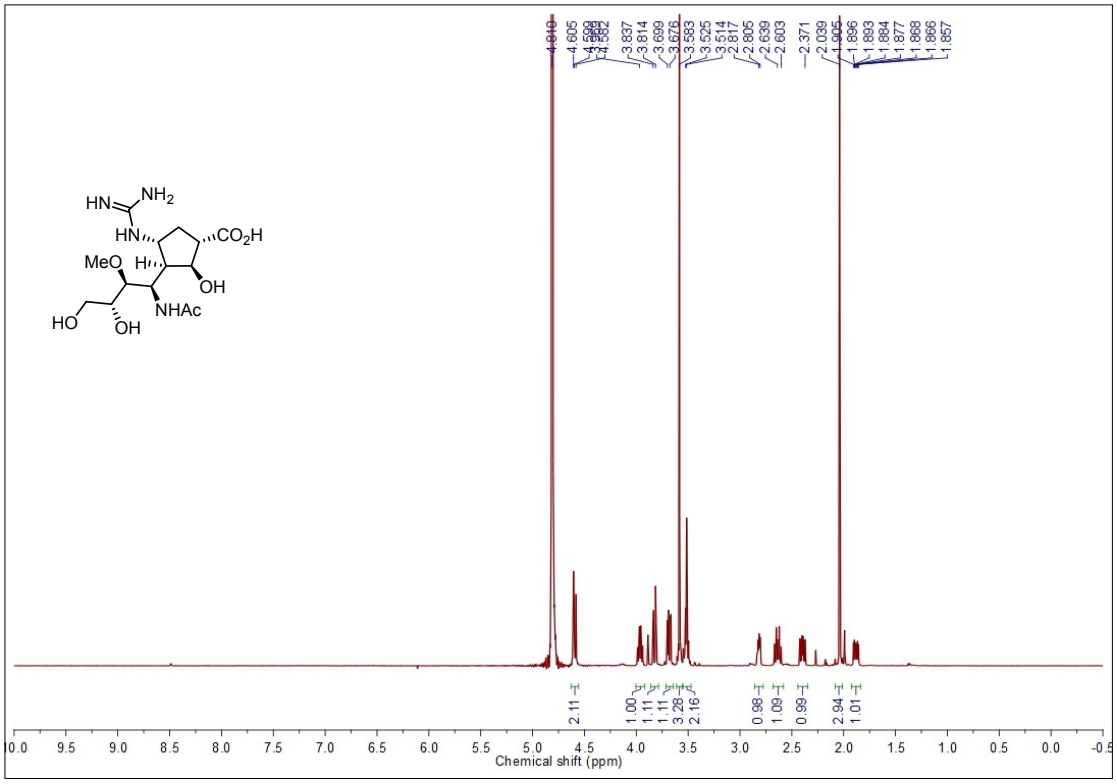


^{13}C NMR spectrum of compound **5** (100 MHz, CD_3OD)

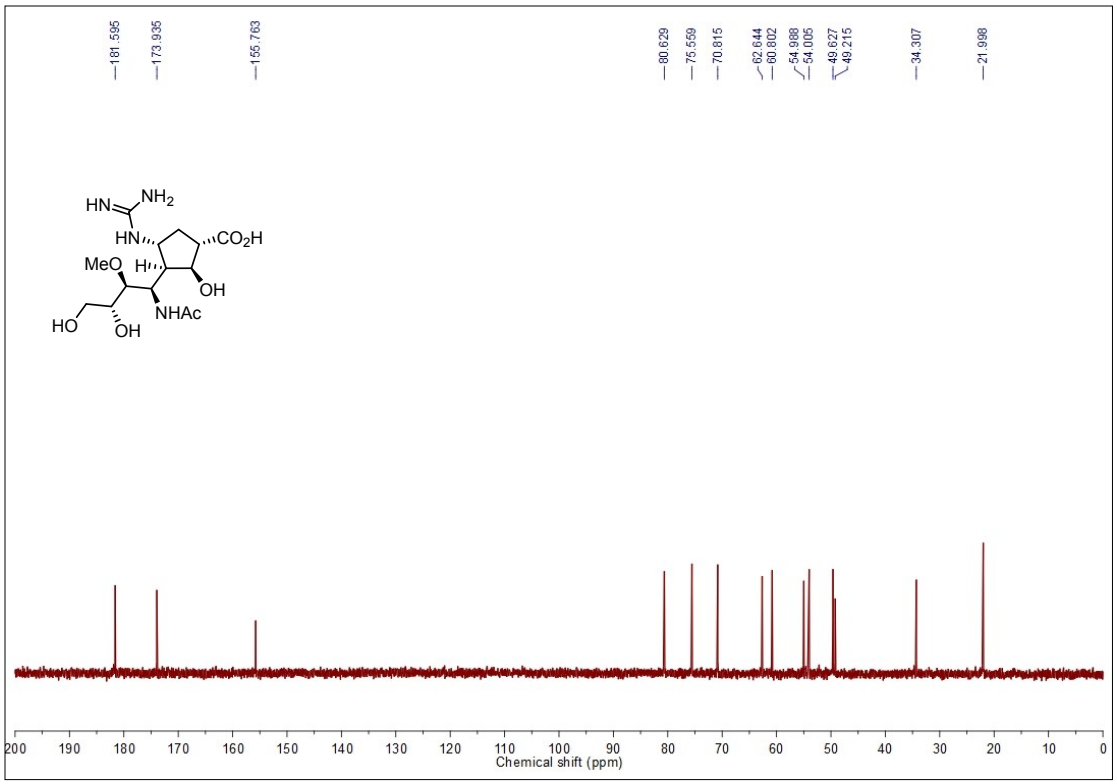


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	2.171	MM	0.0861	2987.29077	578.17151	96.4880
2	3.246	MM	0.2403	108.73340	7.54134	3.5120
Totals :				3096.02417	585.71285	

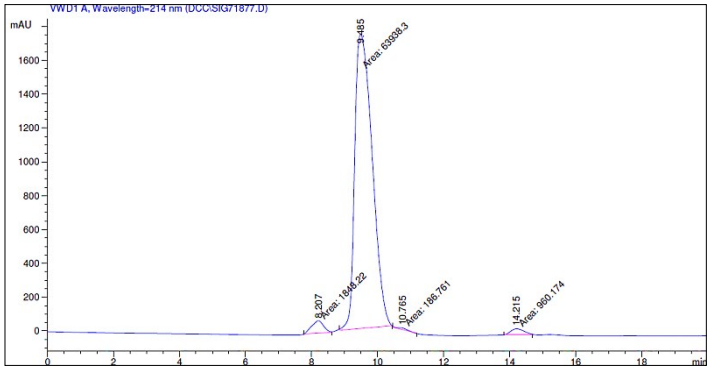
HPLC diagram of compound **5**. HC-C18 column (Agilent, 4.6 × 250 mm, 5 μm particle size), t_R = 2.2 min (elution with water at a flow rate of 0.8 mL/min).



^{1}H NMR spectrum of compound **6** (500 MHz, in D_2O)



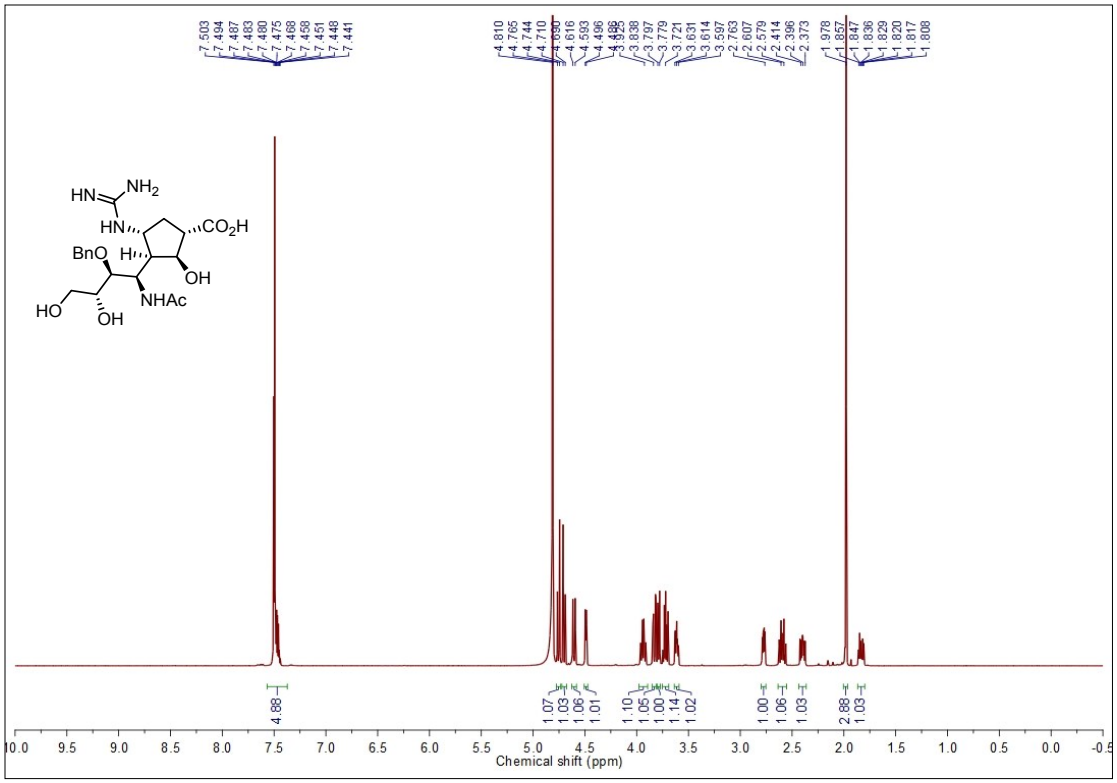
^{13}C NMR spectrum of compound **6** (125 MHz, in D_2O)



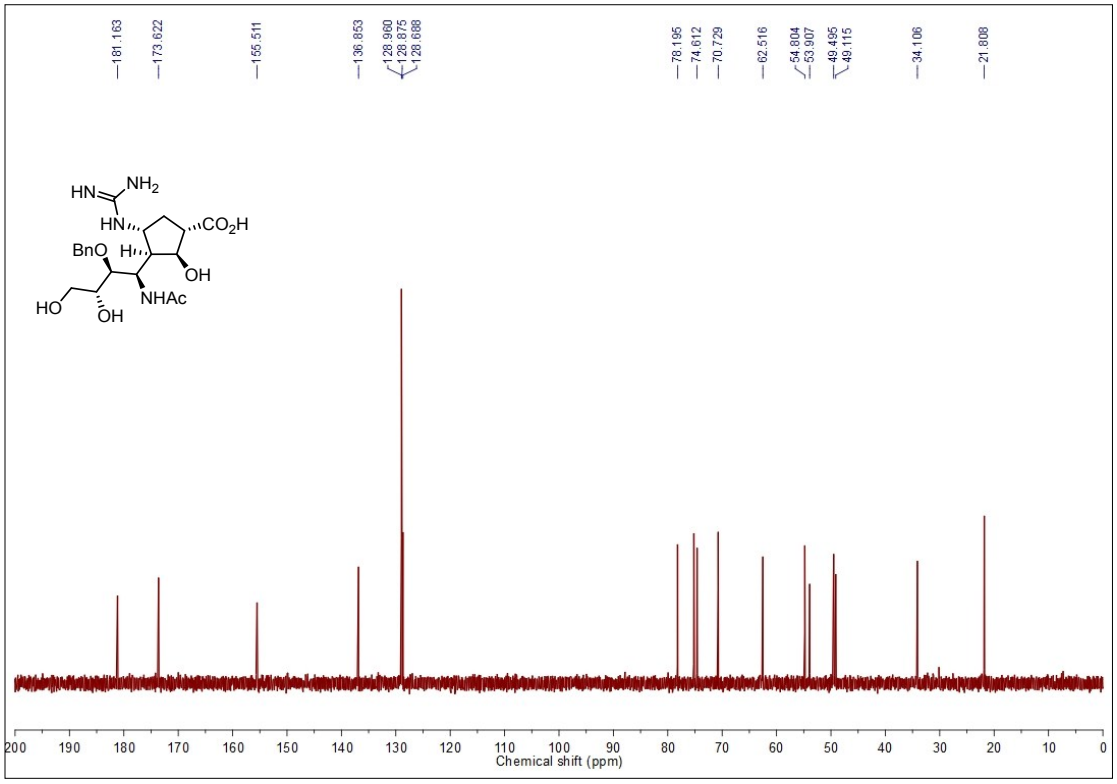
Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.207	MM	0.4204	1848.21851	73.26519	2.7613
2	9.485	MM	0.6124	6.39383e4	1740.23804	95.5252
3	10.765	MM	0.3712	186.76120	9.28727	0.2790
4	14.215	MM	0.4613	960.17407	34.69242	1.4345
Totals :				6.69334e4	1857.48292	

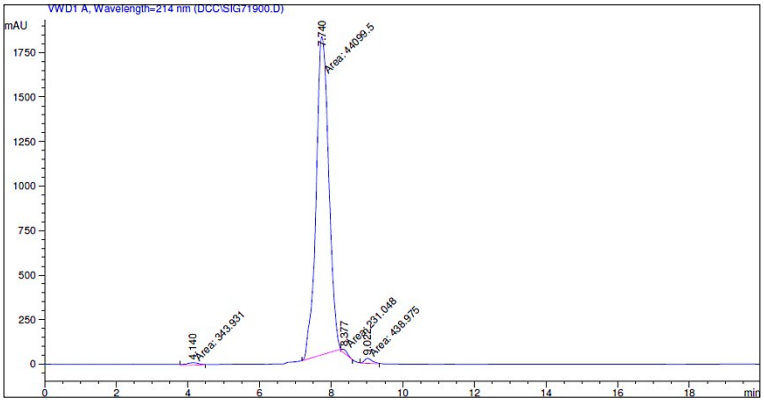
HPLC diagram of compound **6**. HC-C18 column (Agilent, 4.6 × 250 mm, 5 μm particle size), t_R = 9.5 min (elution with 0.25 M NH_4HCO_3 aqueous solution at a flow rate of 0.2 mL/min).



^{1}H NMR spectrum of compound **7** (500 MHz, in D_2O)



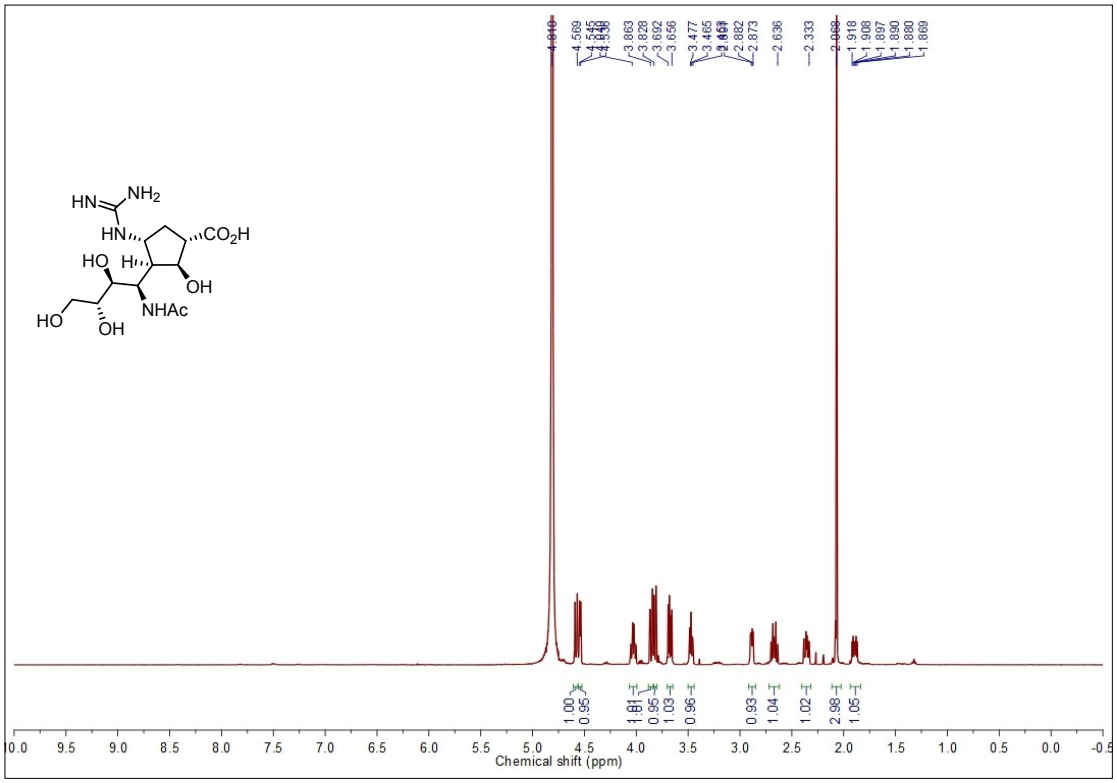
^{13}C NMR spectrum of compound **7** (125 MHz, in D_2O)



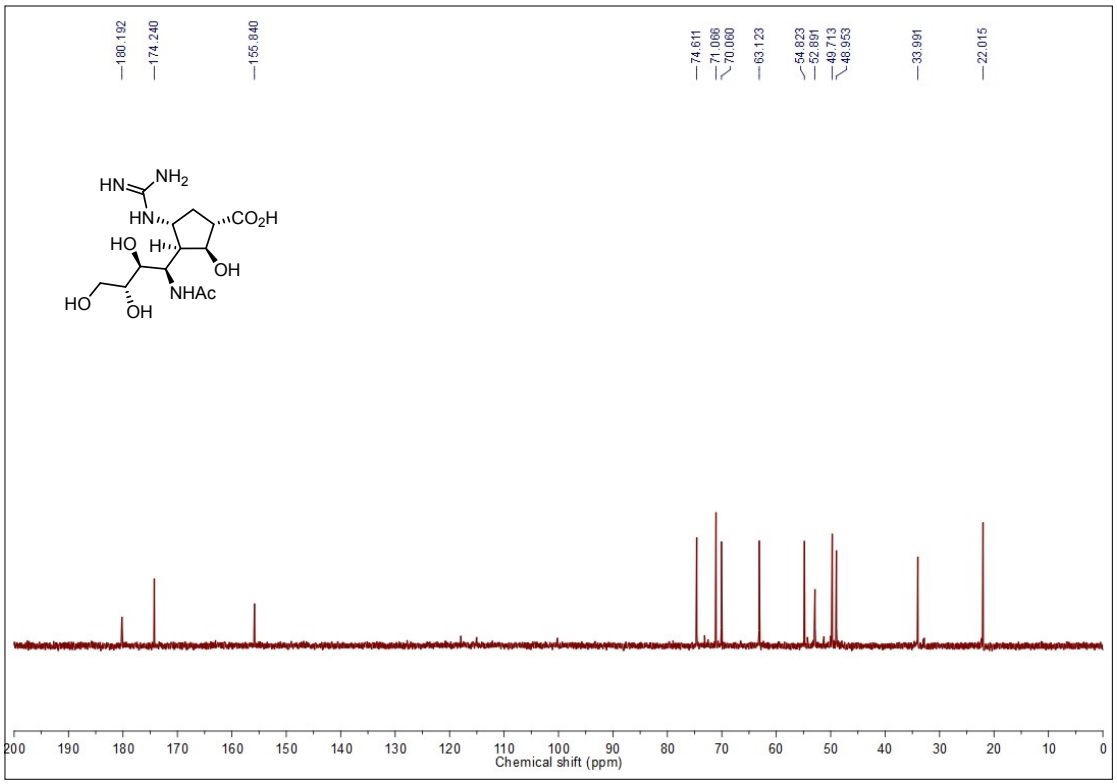
Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.140	MM	0.4343	343.93060	13.19944	0.7624
2	7.740	MM	0.4109	4.40995e4	1788.75085	97.7524
3	8.377	MM	0.1805	231.04762	21.33582	0.5121
4	9.022	MM	0.2557	438.97473	28.61784	0.9730
Totals :				4.51135e4	1851.90396	

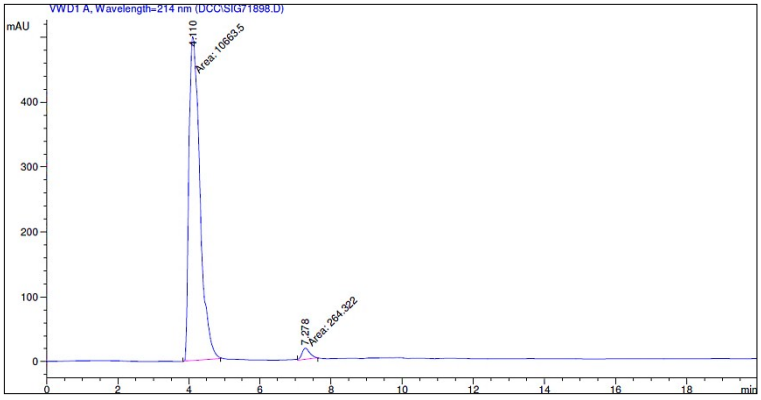
HPLC diagram of compound **7**. HC-C18 column (Agilent, 4.6 × 250 mm, 5 μm particle size), t_R = 7.7 min (elution with MeOH/H_2O = 3:17 at a flow rate of 0.4 mL/min).



^{1}H NMR spectrum of compound **8** (500 MHz, in D_2O)



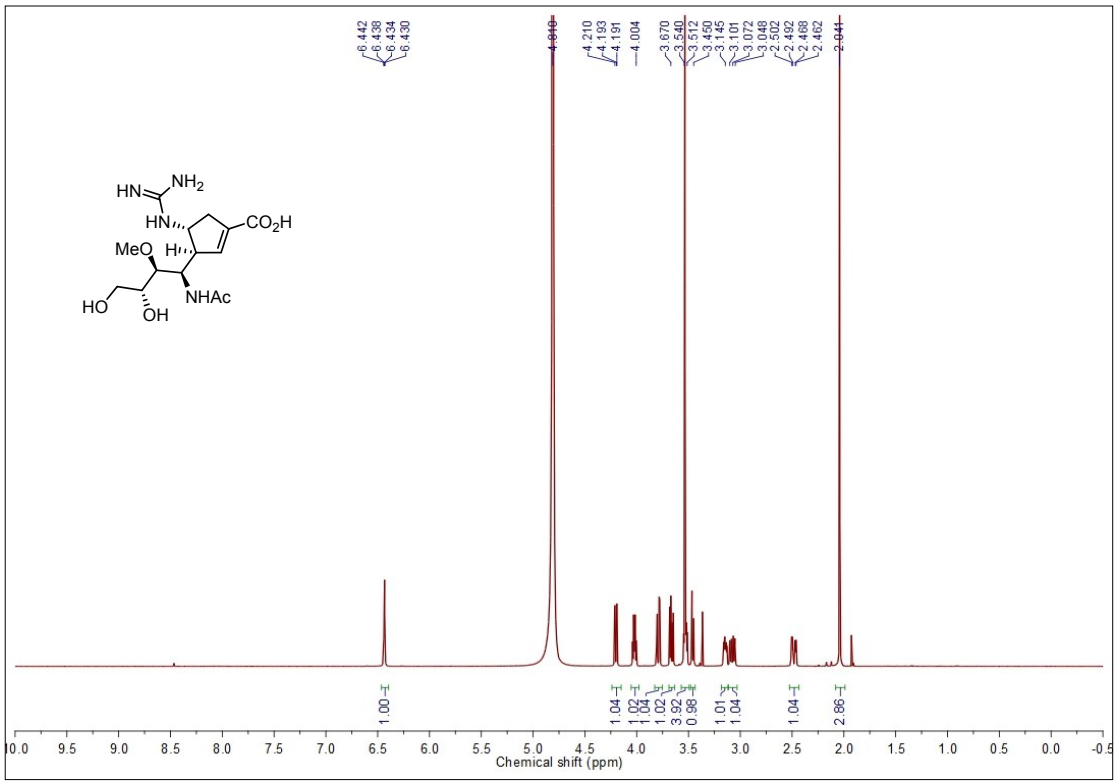
^{13}C NMR spectrum of compound **8** (100 MHz, in D_2O)



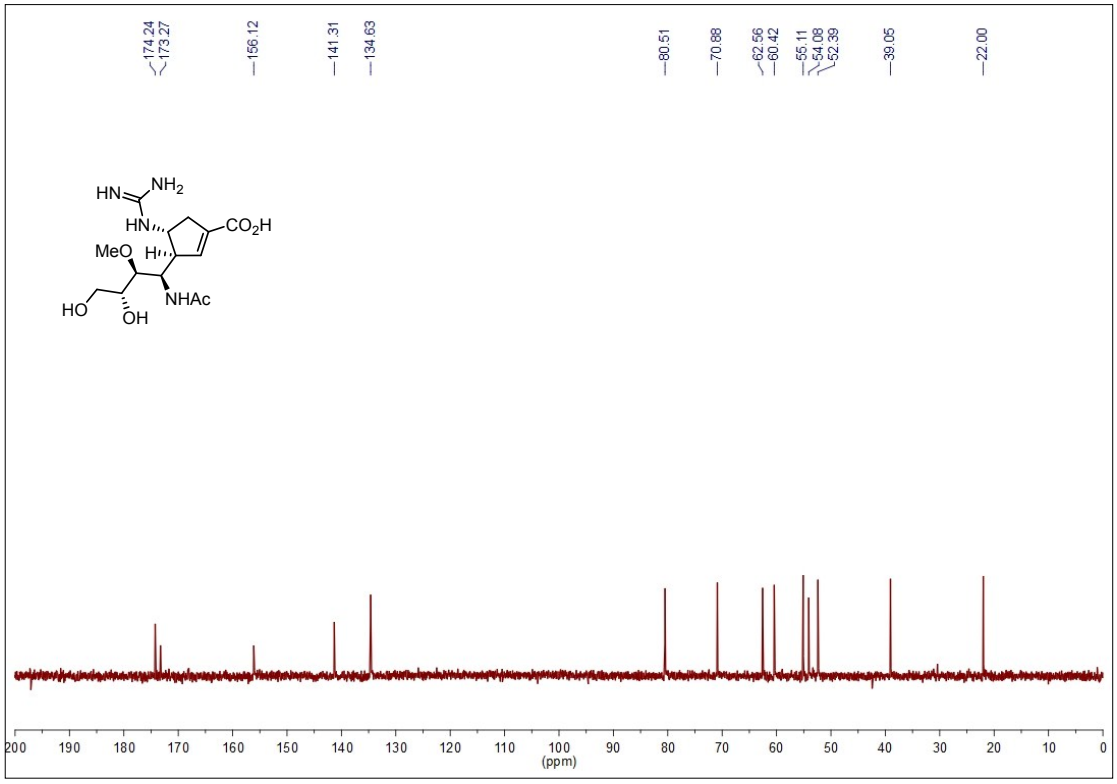
Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	4.110	MM	0.3560	1.06635e4	499.26108	97.5812
2	7.278	MM	0.2557	264.32166	17.23073	2.4188
Totals :				1.09278e4	516.49181	

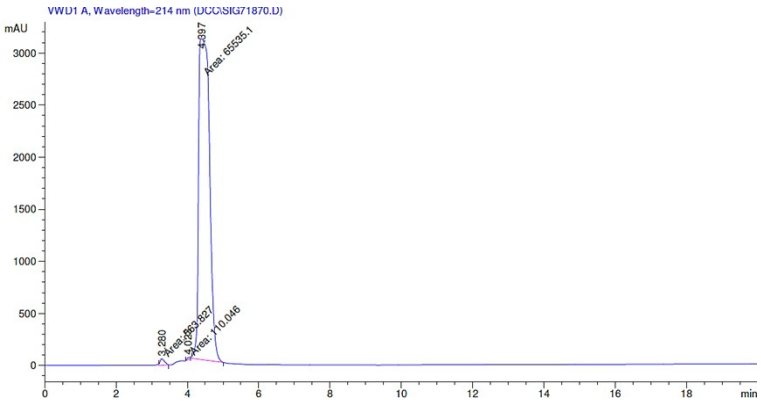
HPLC diagram of compound **8**. HC-C18 column (Agilent, 4.6 × 250 mm, 5 µm particle size), t_R = 4.1 min [MeOH/H_2O = 3:17] at a flow rate of 0.4 mL/min.



^{1}H NMR spectrum of compound **9** (500 MHz, in D_2O)



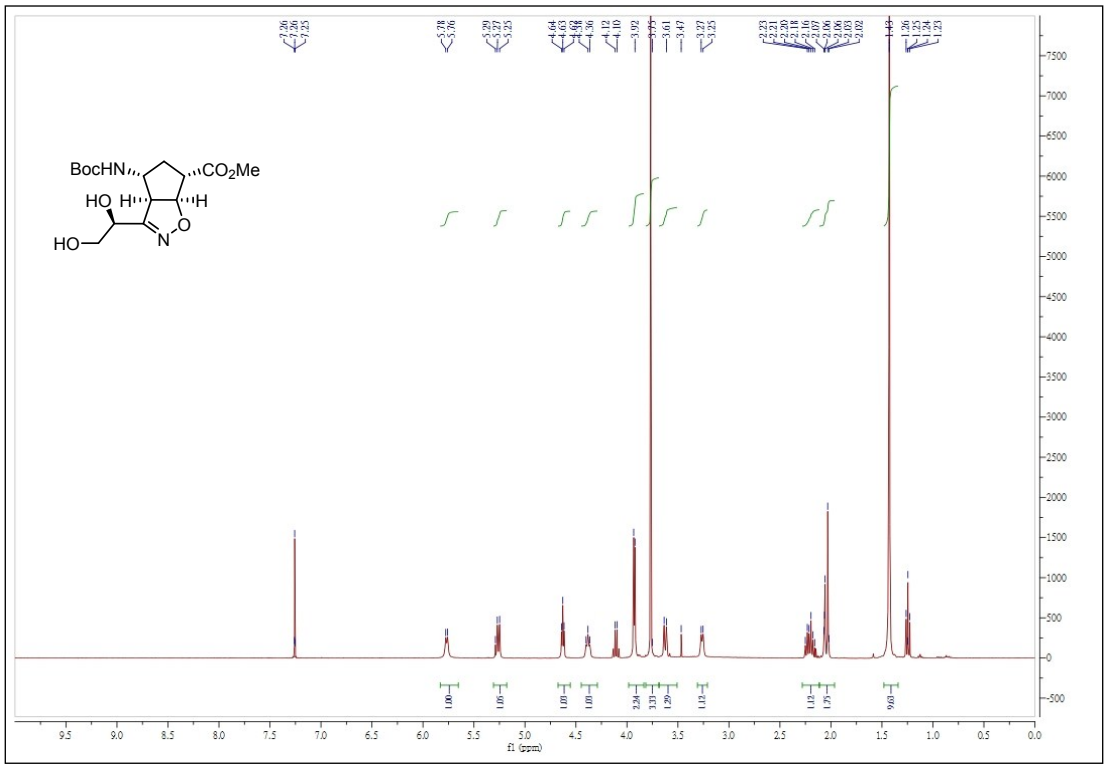
^{13}C NMR spectrum of compound **9** (100 MHz, in D_2O)



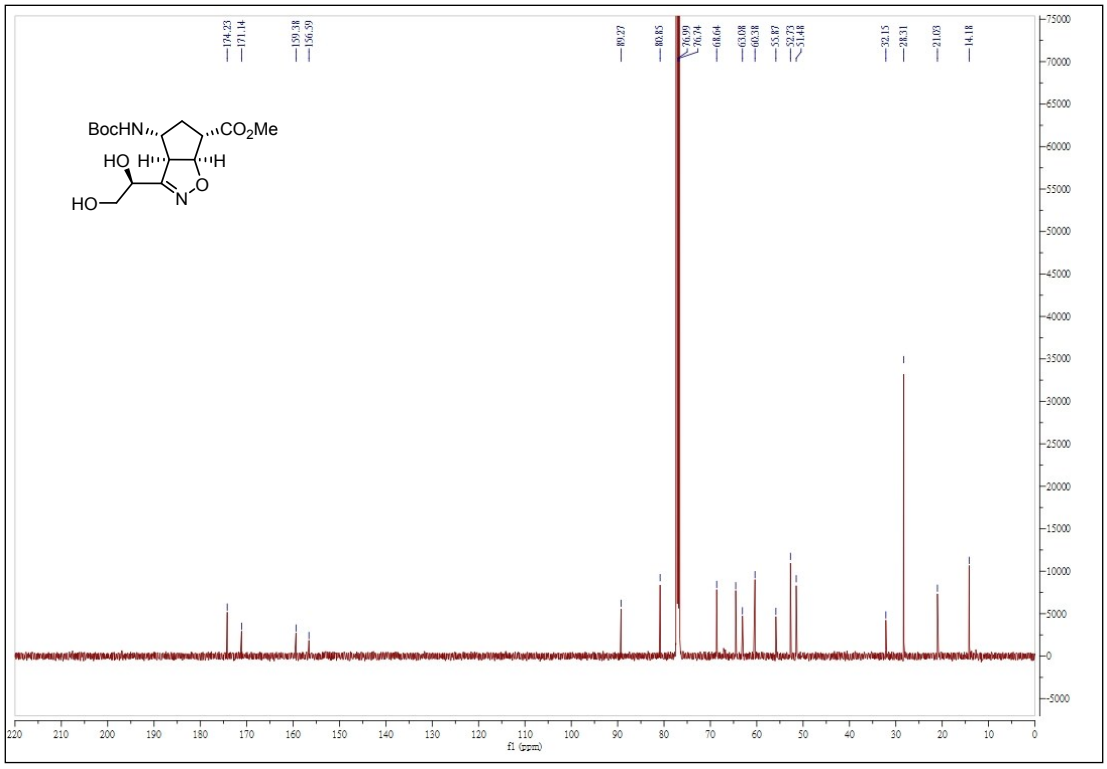
Signal 1: VWD1 A, Wavelength=214 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	3.280	MM	0.1456	563.82739	64.52071	0.8516
2	4.023	MM	0.0964	110.04555	19.02506	0.1662
3	4.397	MM	0.3544	6.55351e4	3081.85352	98.9822
Totals :				6.62089e4	3165.39928	

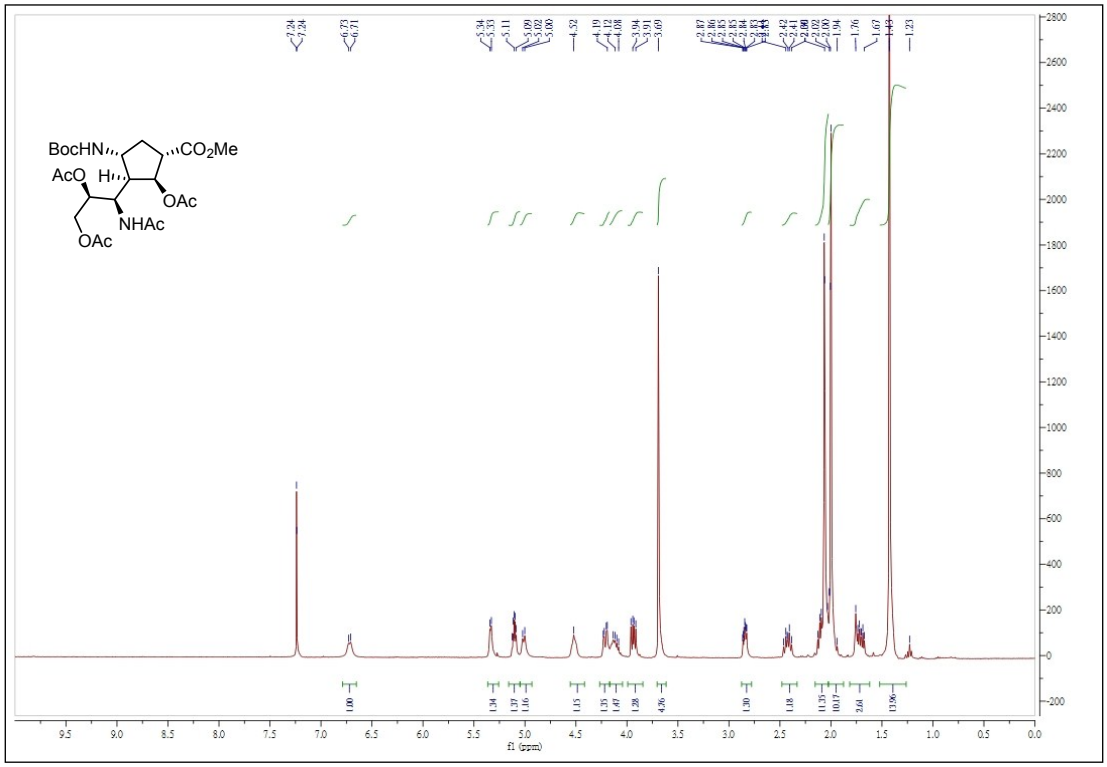
HPLC diagram of compound **9**. HC-C18 column (Agilent, 4.6 × 250 mm, 5 μm particle size), t_R = 4.4 min [0.25 M NH_4HCO_3 aqueous solution] at a flow rate of 0.5 mL/min.



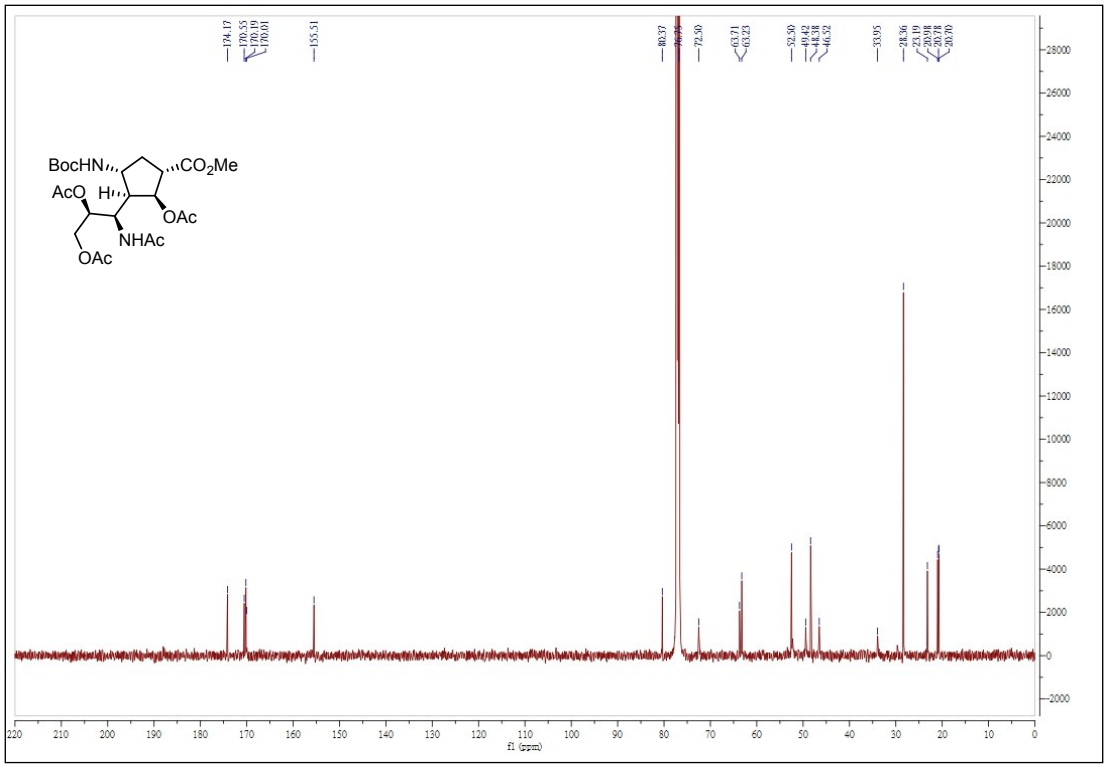
^{1}H NMR spectrum of compound **12** (400 MHz, $CDCl_3$)



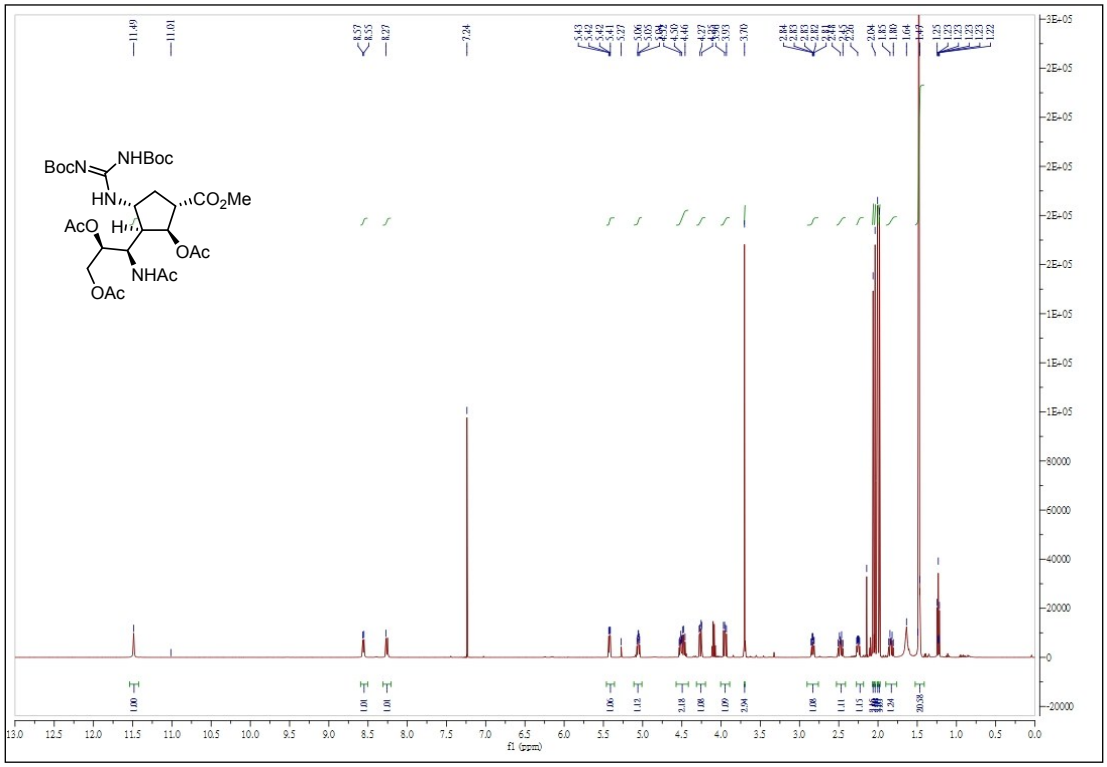
^{13}C NMR spectrum of compound **12** (125 MHz, $CDCl_3$)



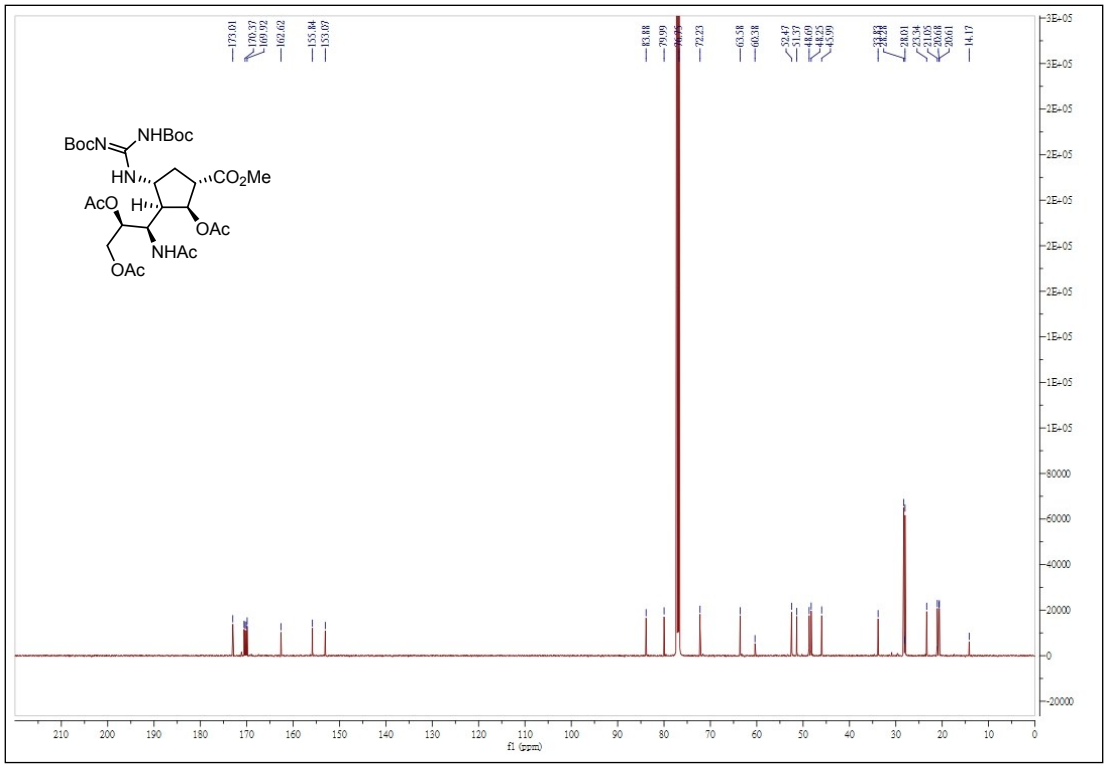
^{1}H NMR spectrum of compound **13** (500 MHz, $CDCl_3$)



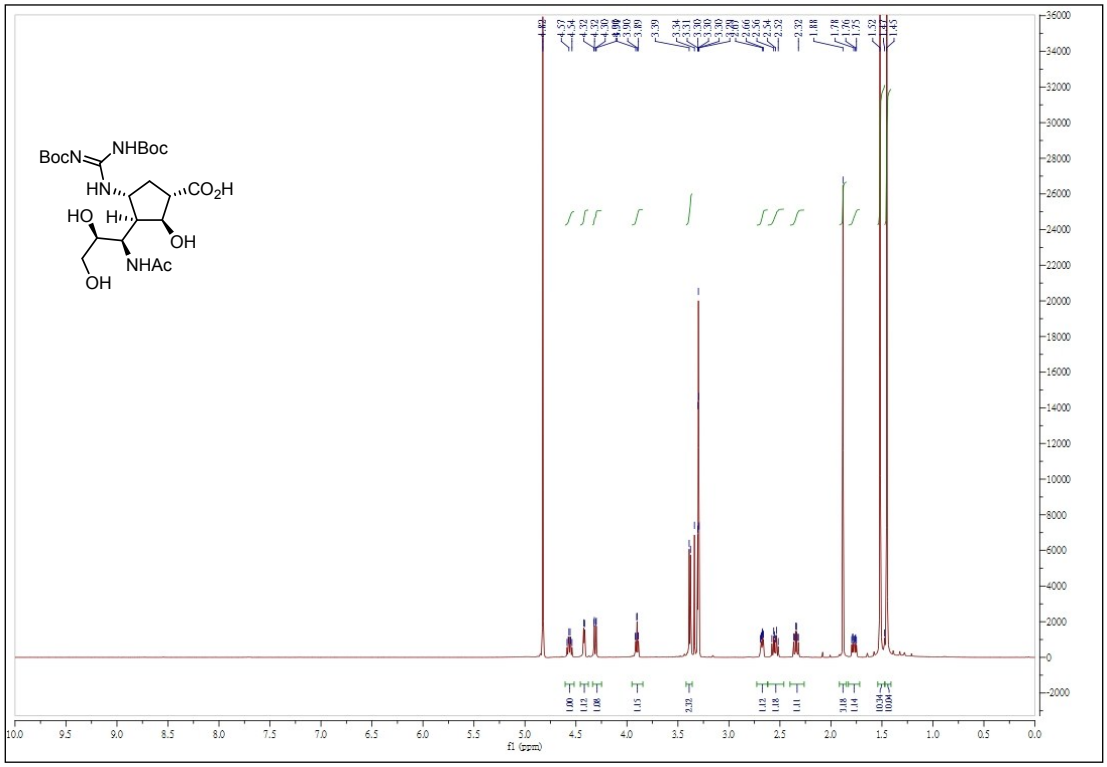
^{13}C NMR spectrum of compound **13** (125 MHz, $CDCl_3$)



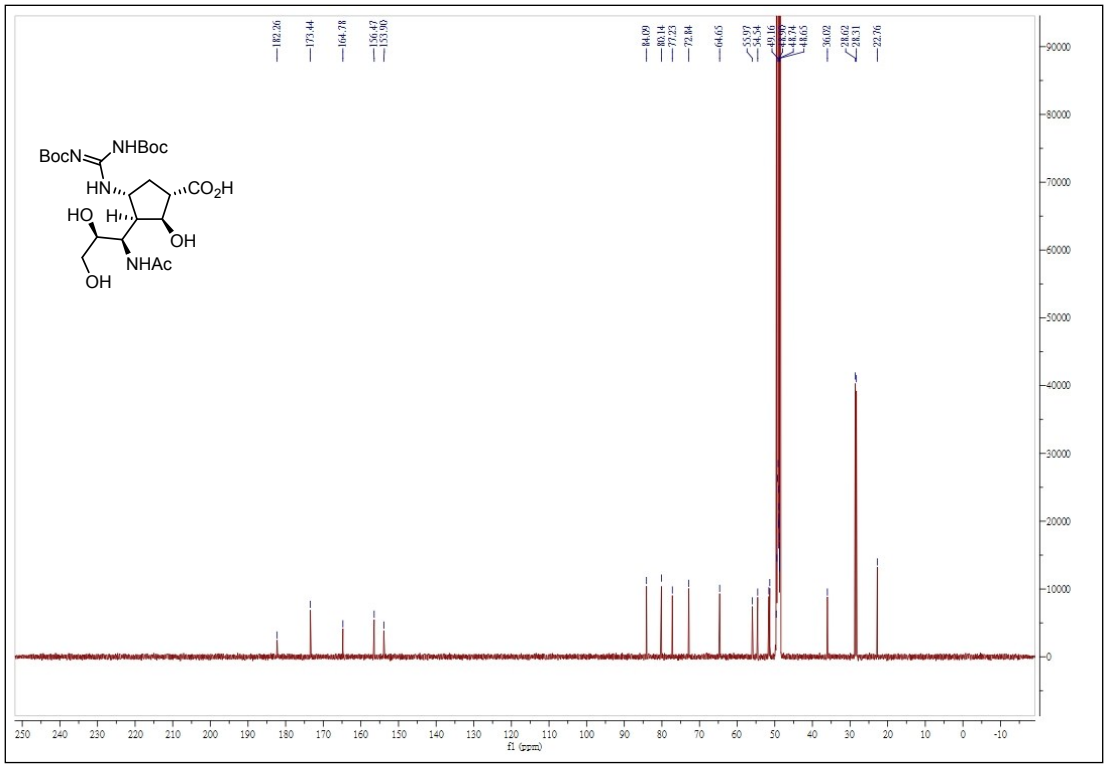
^{1}H NMR spectrum of compound **14** (500 MHz, $CDCl_3$)



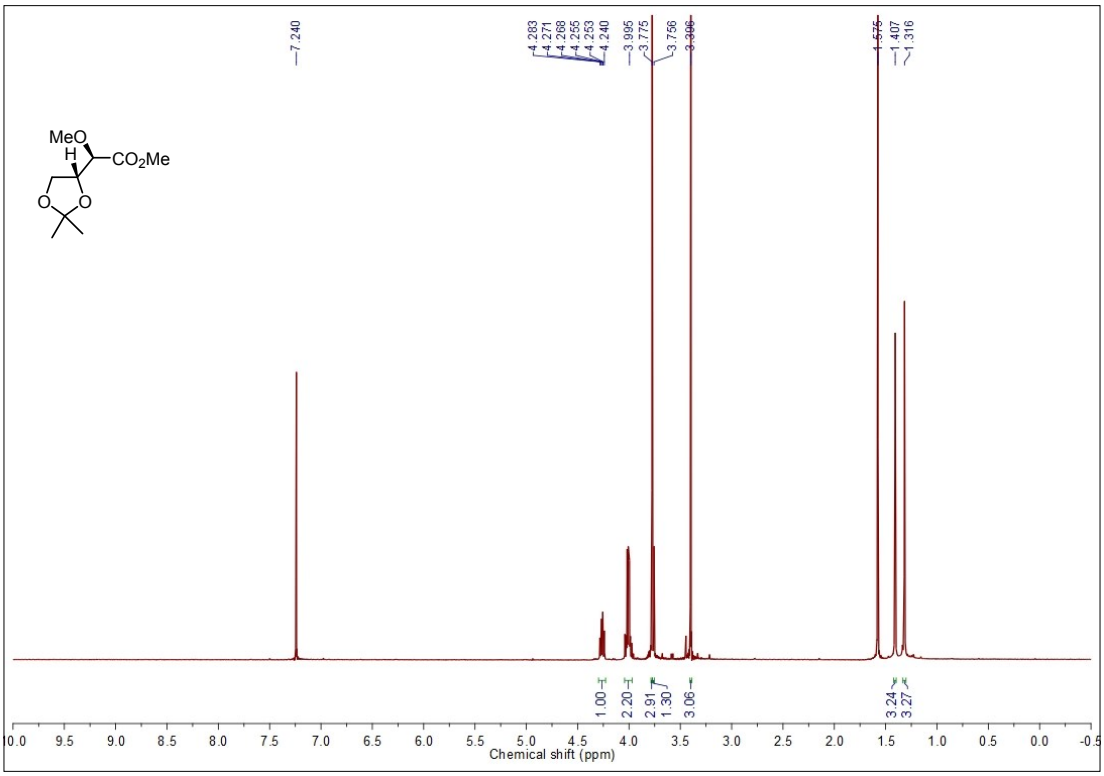
^{13}C NMR spectrum of compound **14** (125 MHz, $CDCl_3$)



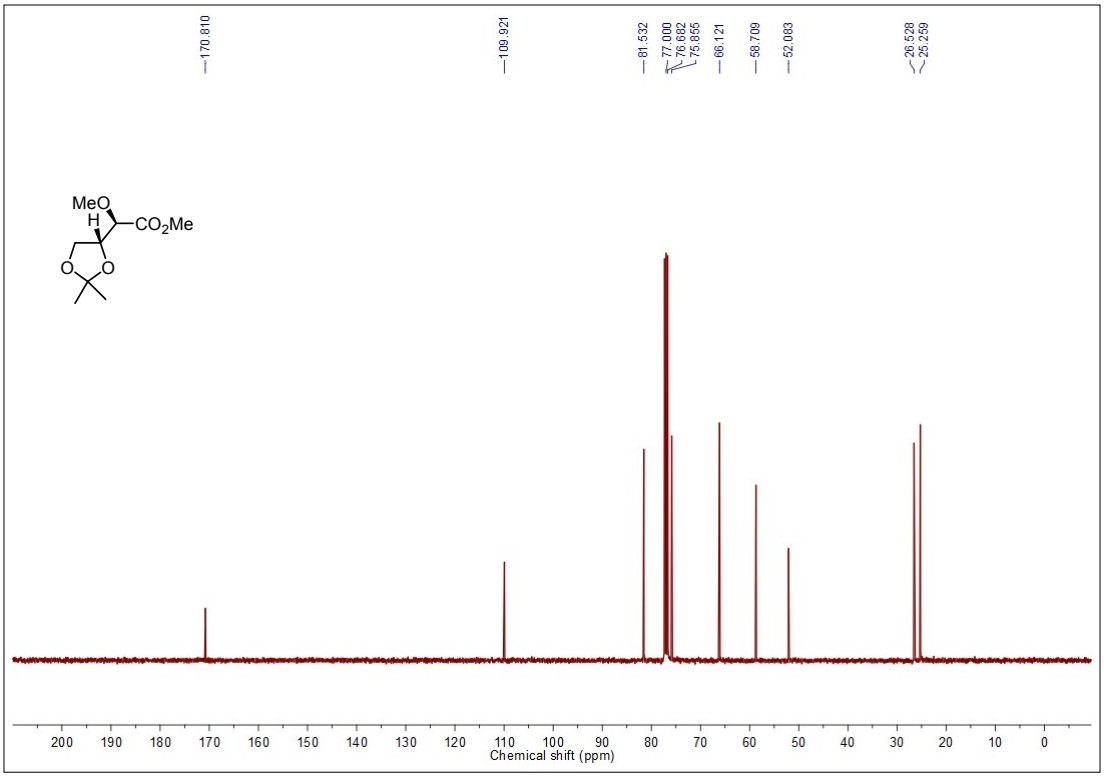
^{1}H NMR spectrum of compound **15** (500 MHz, CD_3OD)



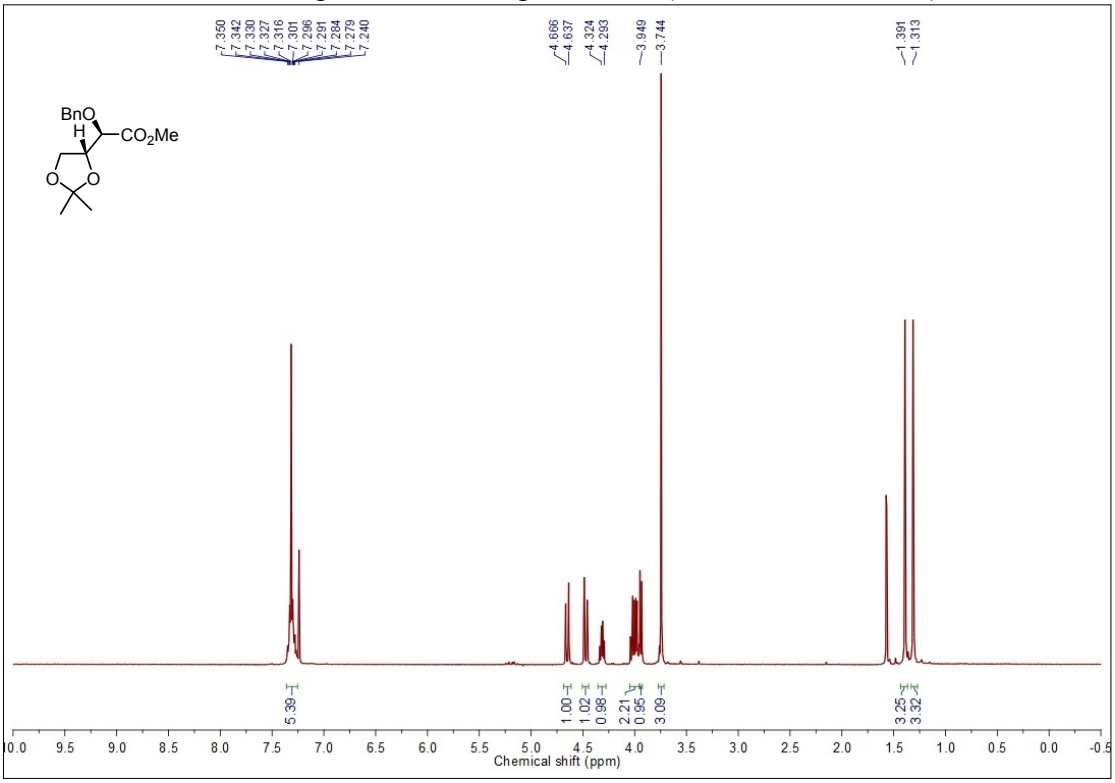
^{13}C NMR spectrum of compound **15** (125 MHz, CD_3OD)



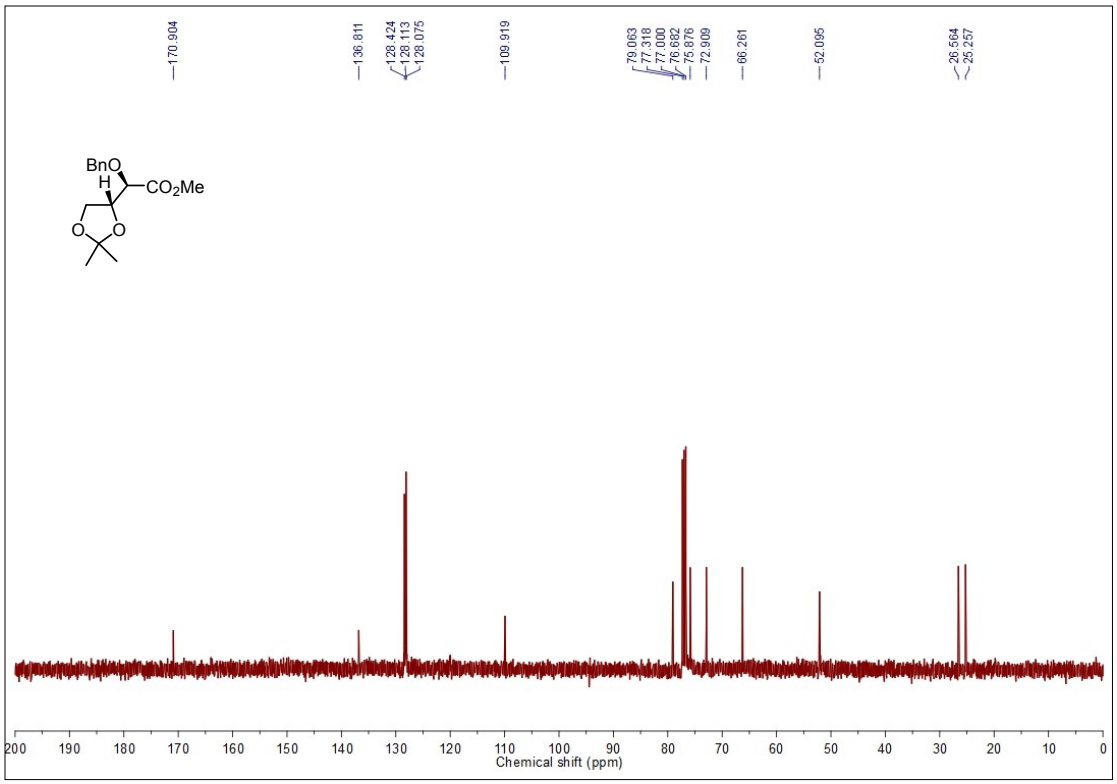
^{1}H NMR spectrum of compound **17a** (400 MHz, in $CDCl_3$)



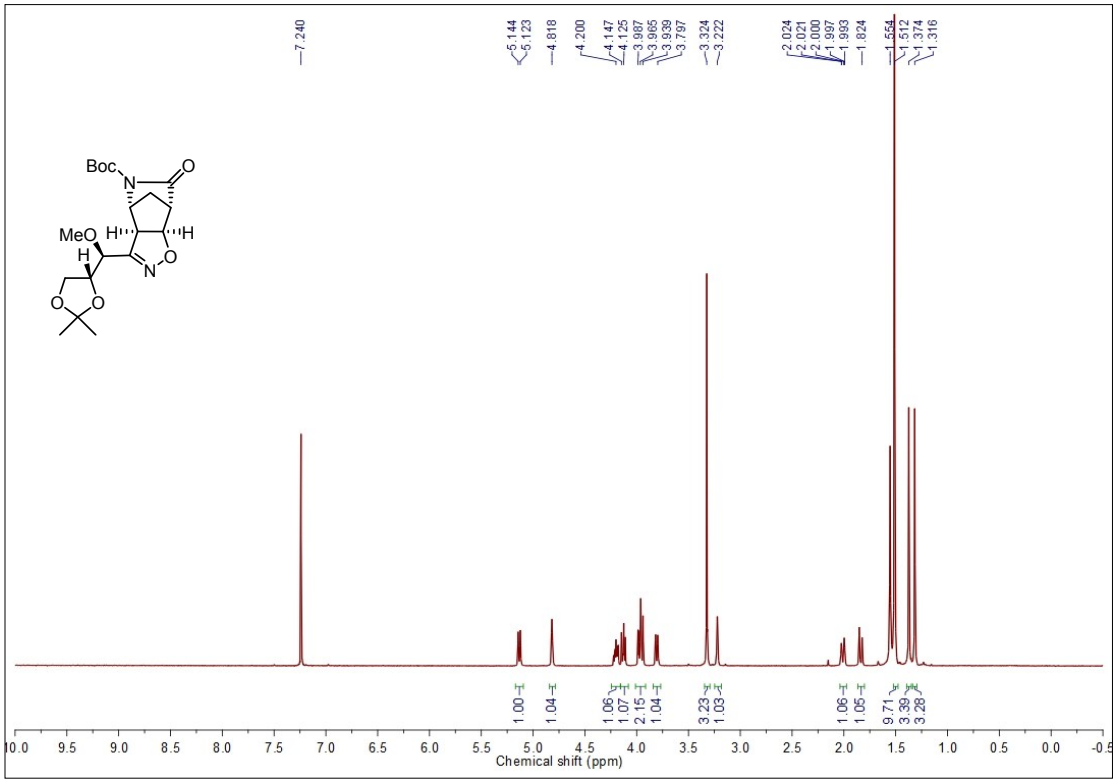
^{13}C NMR spectrum of compound **17a** (100 MHz, in $CDCl_3$)



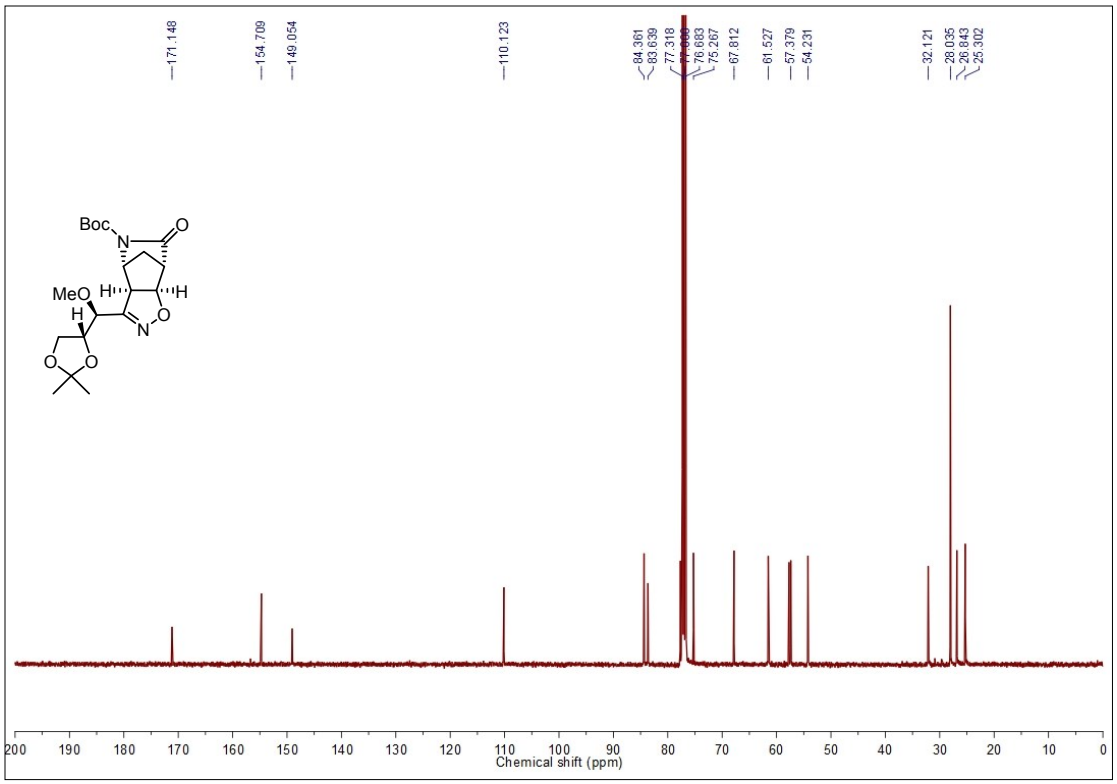
^{1}H NMR spectrum of compound **17b** (400 MHz, in $CDCl_3$)



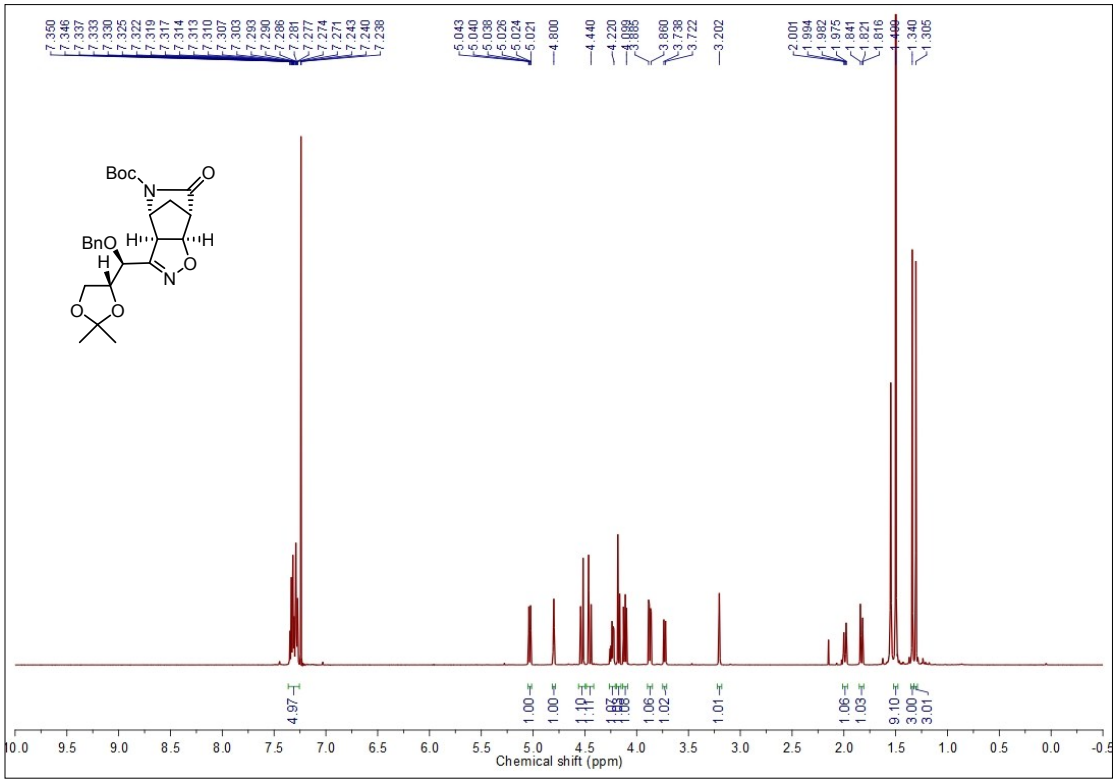
^{13}C NMR spectrum of compound **17b** (100 MHz, in $CDCl_3$)



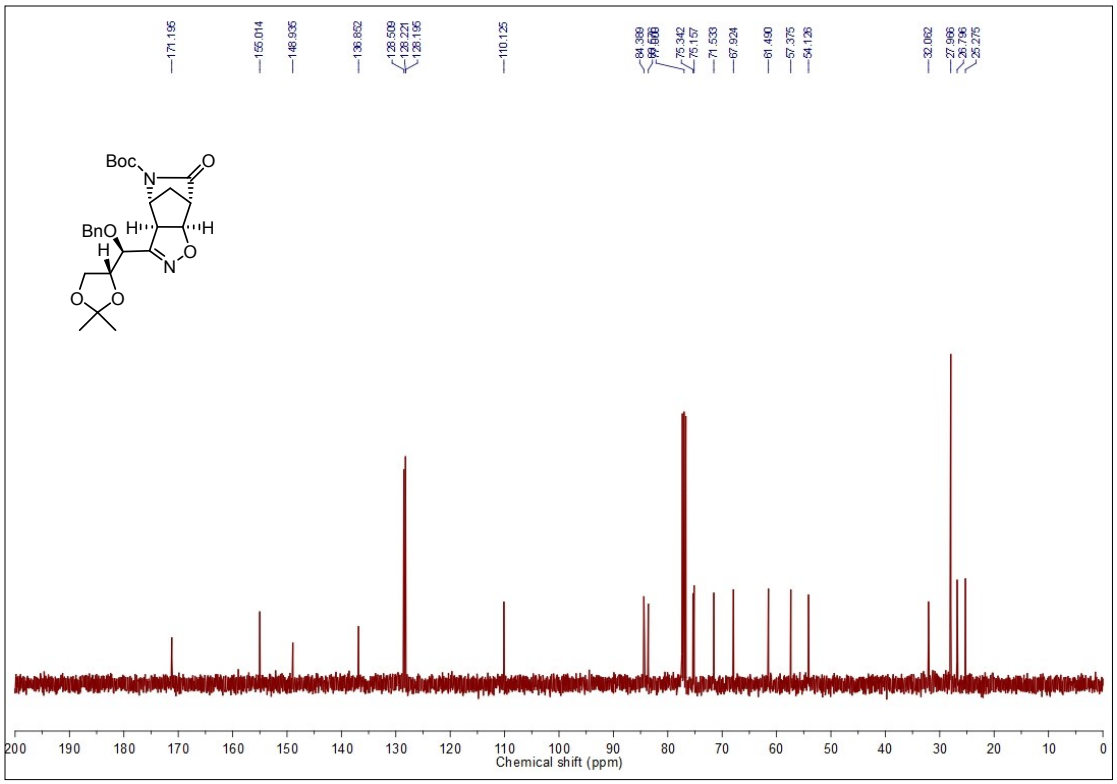
^{1}H NMR spectrum of compound **21a** (500 MHz, in $CDCl_3$)



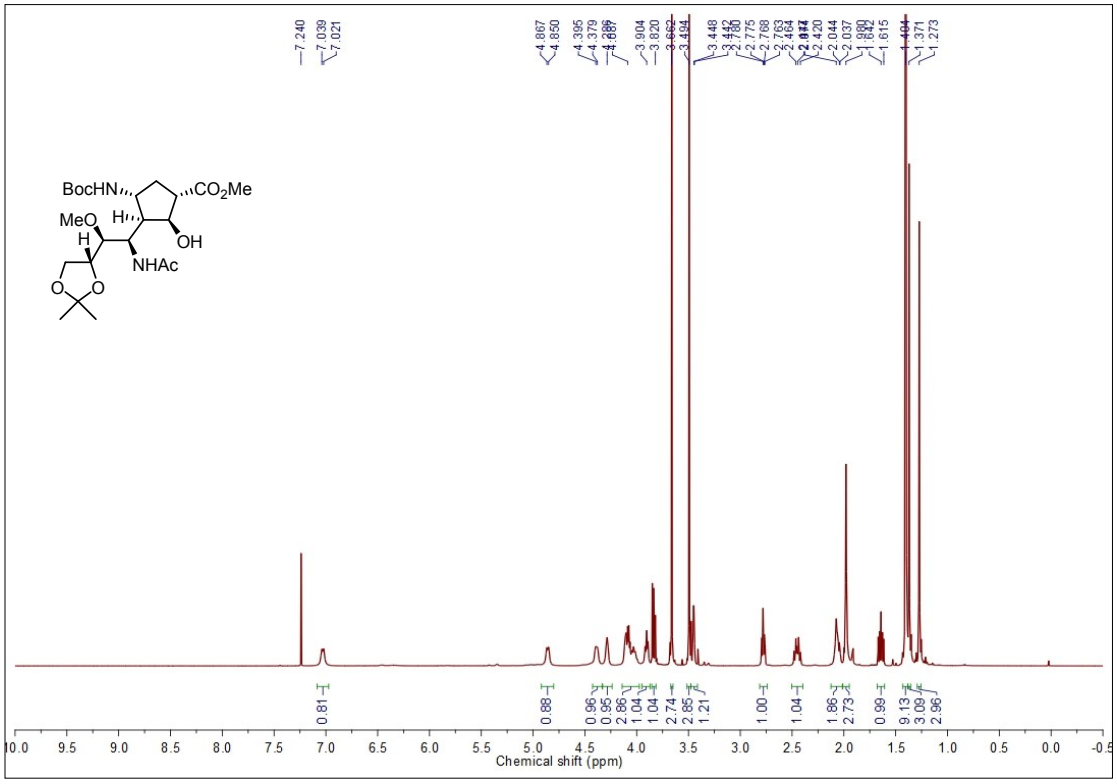
^{13}C NMR spectrum of compound **21a** (125 MHz, in $CDCl_3$)



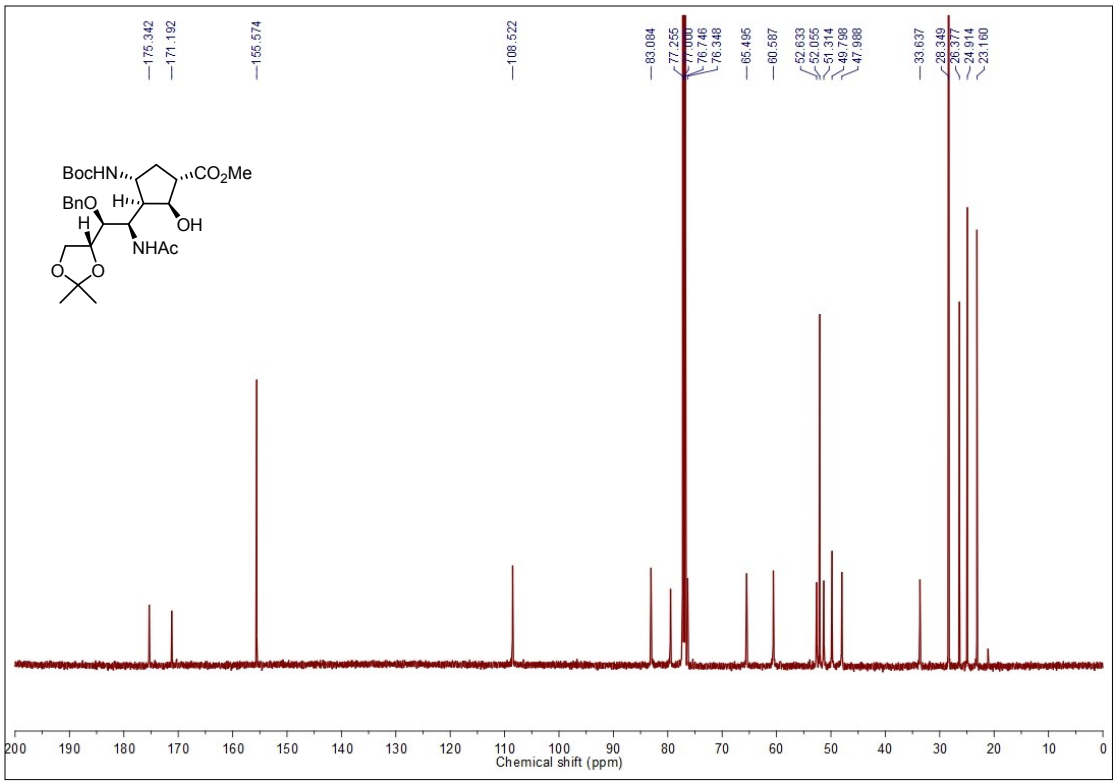
^{1}H NMR spectrum of compound **21b** (500 MHz, in $CDCl_3$)



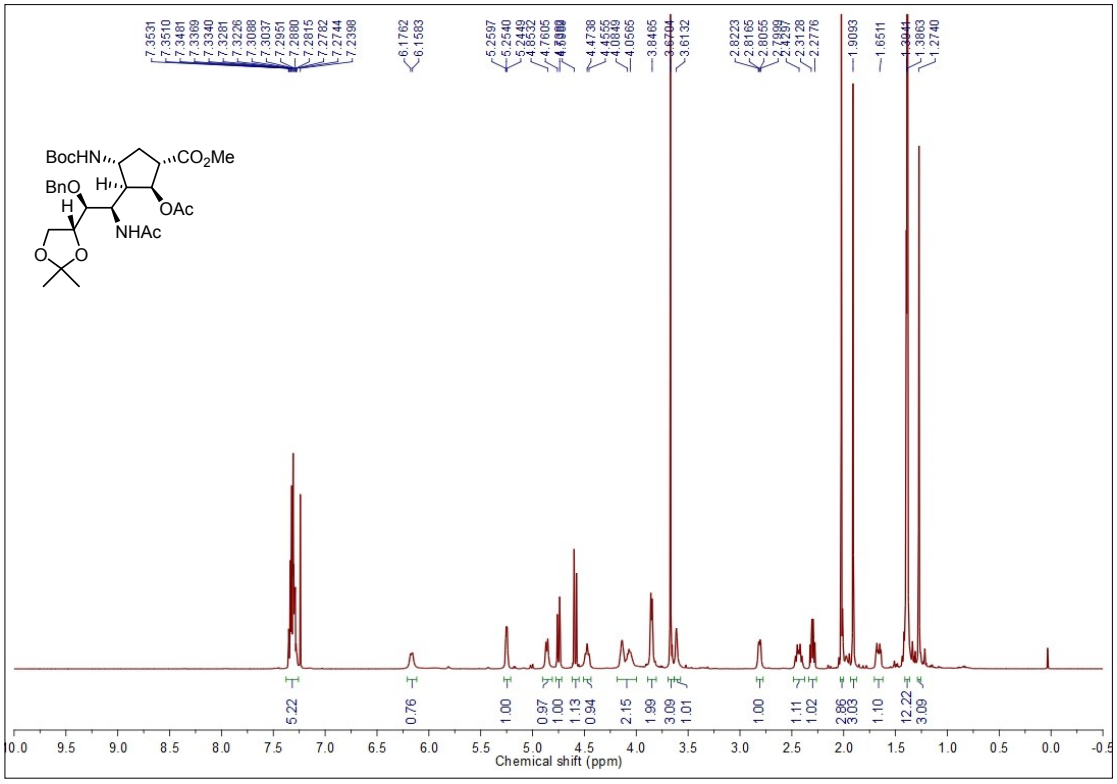
^{13}C NMR spectrum of compound **21b** (100 MHz, in $CDCl_3$)



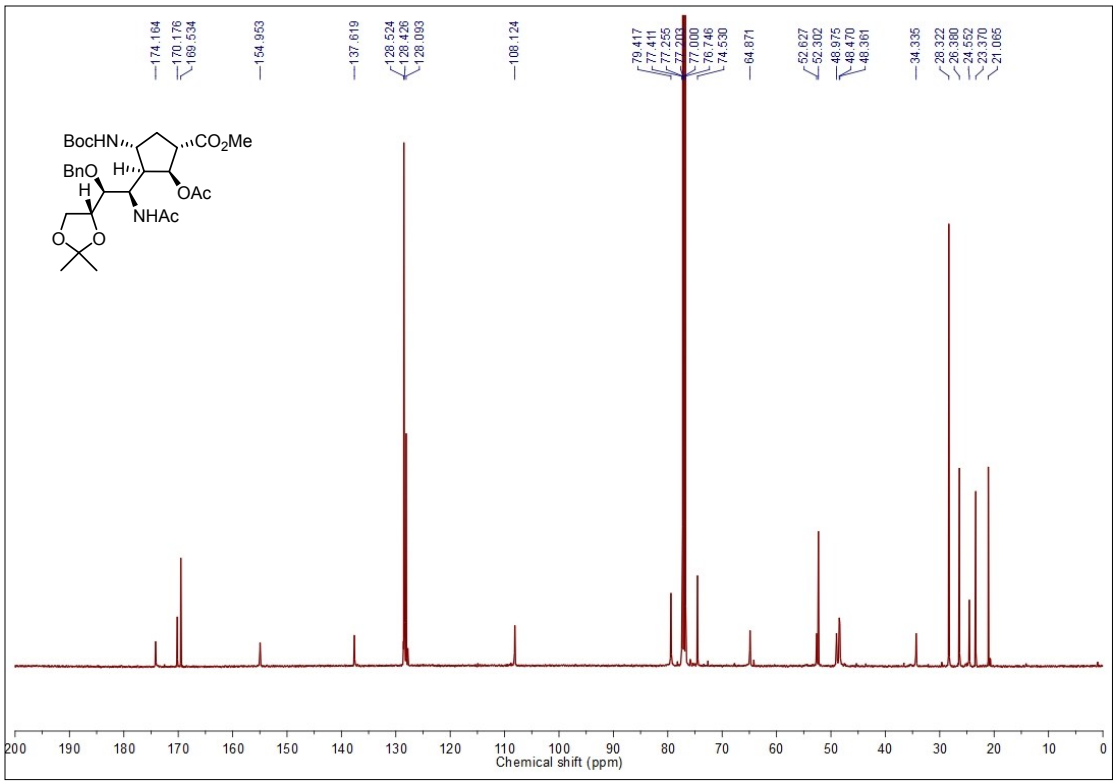
^{1}H NMR spectrum of compound **22a** (500 MHz, in $CDCl_3$)



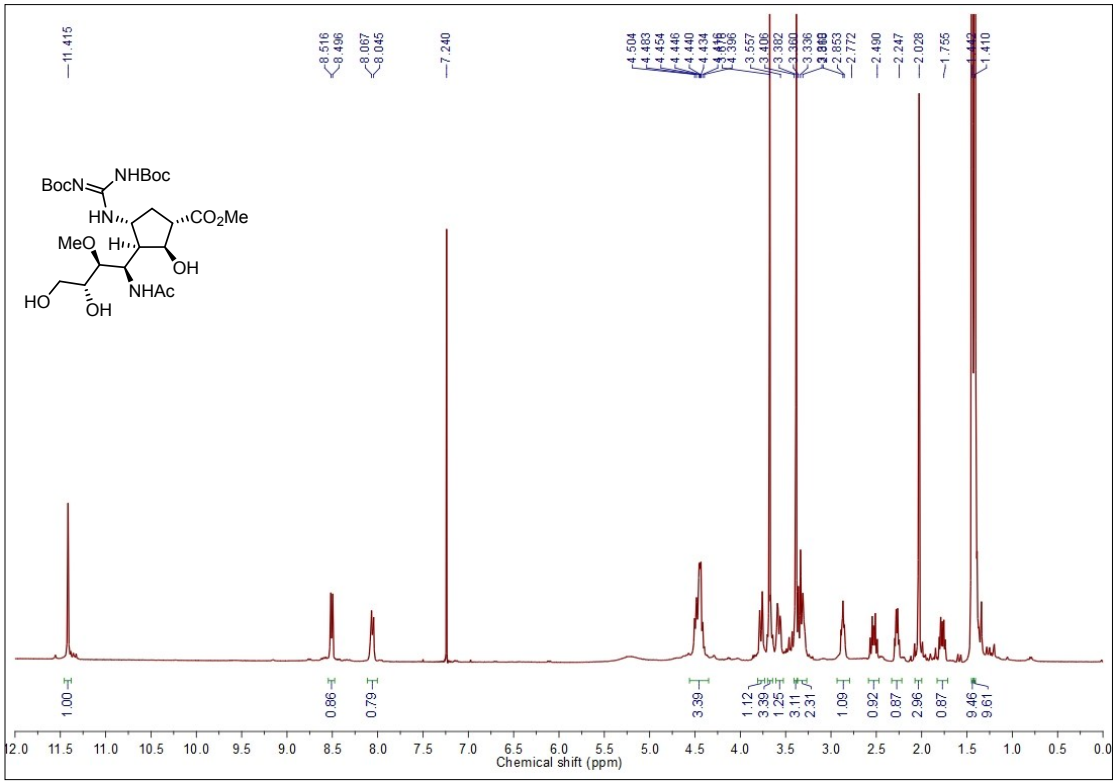
^{13}C NMR spectrum of compound **22a** (125 MHz, in $CDCl_3$)



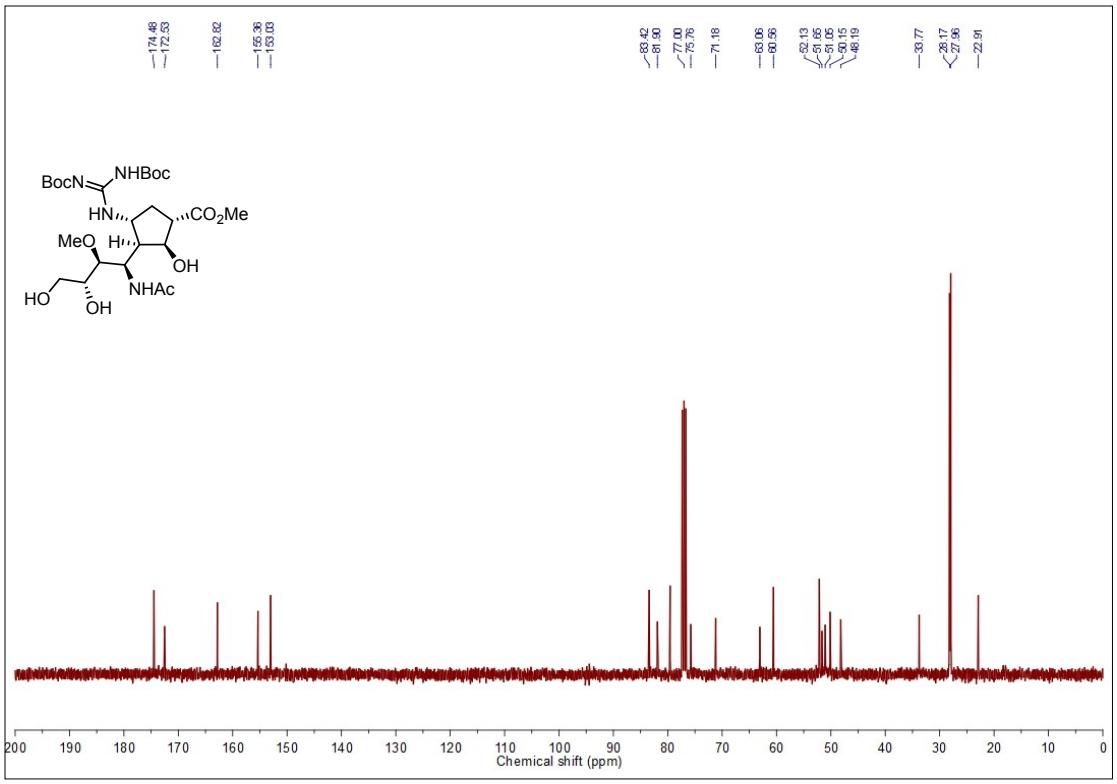
^{1}H NMR spectrum of compound **22b** (500 MHz, in $CDCl_3$)



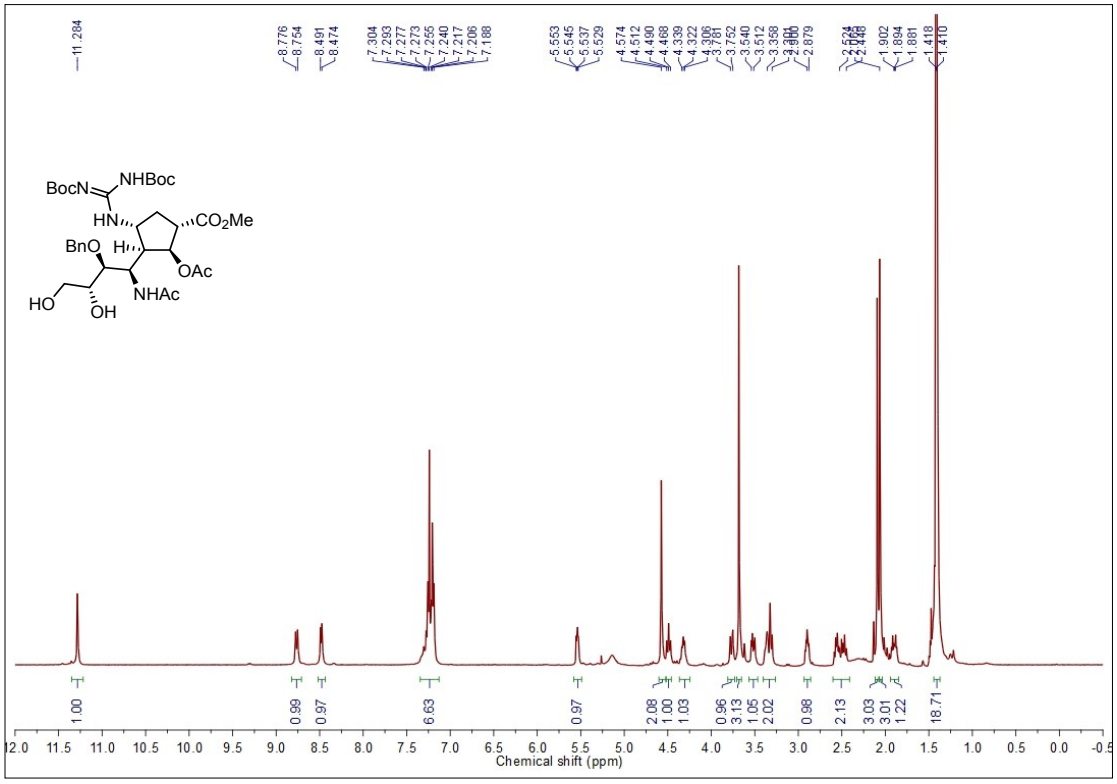
^{13}C NMR spectrum of compound **22b** (125 MHz, in $CDCl_3$)



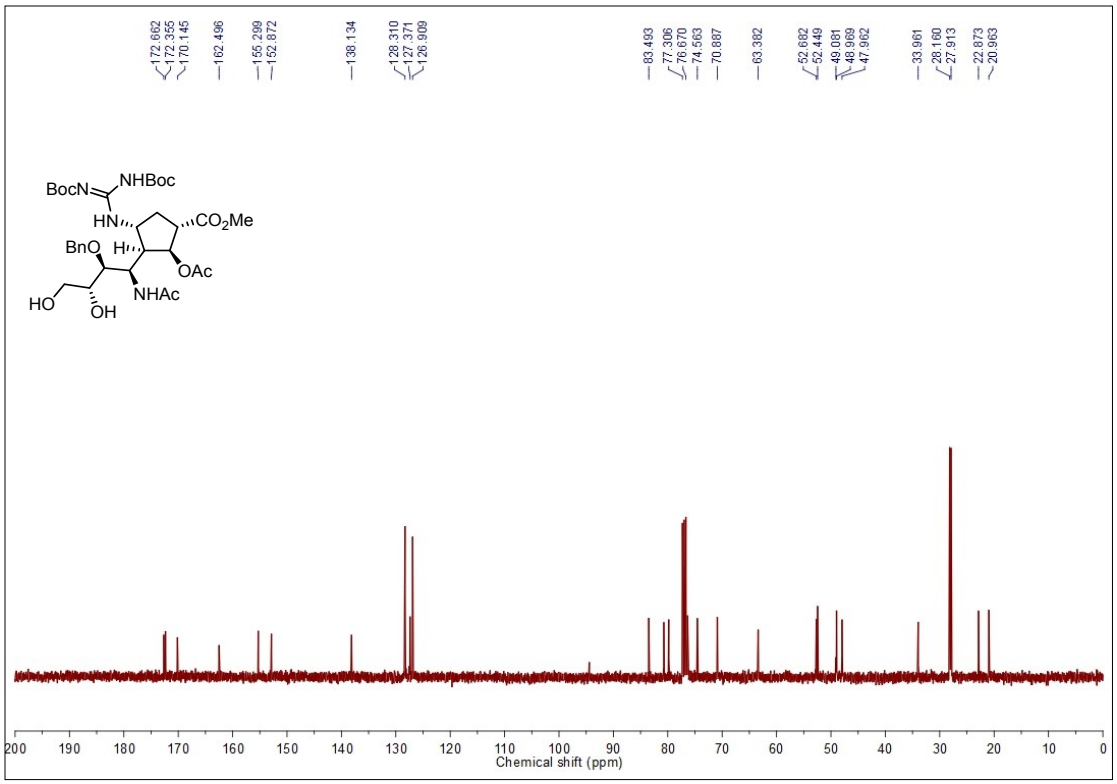
^{1}H NMR spectrum of compound **23a** (400 MHz, in $CDCl_3$)



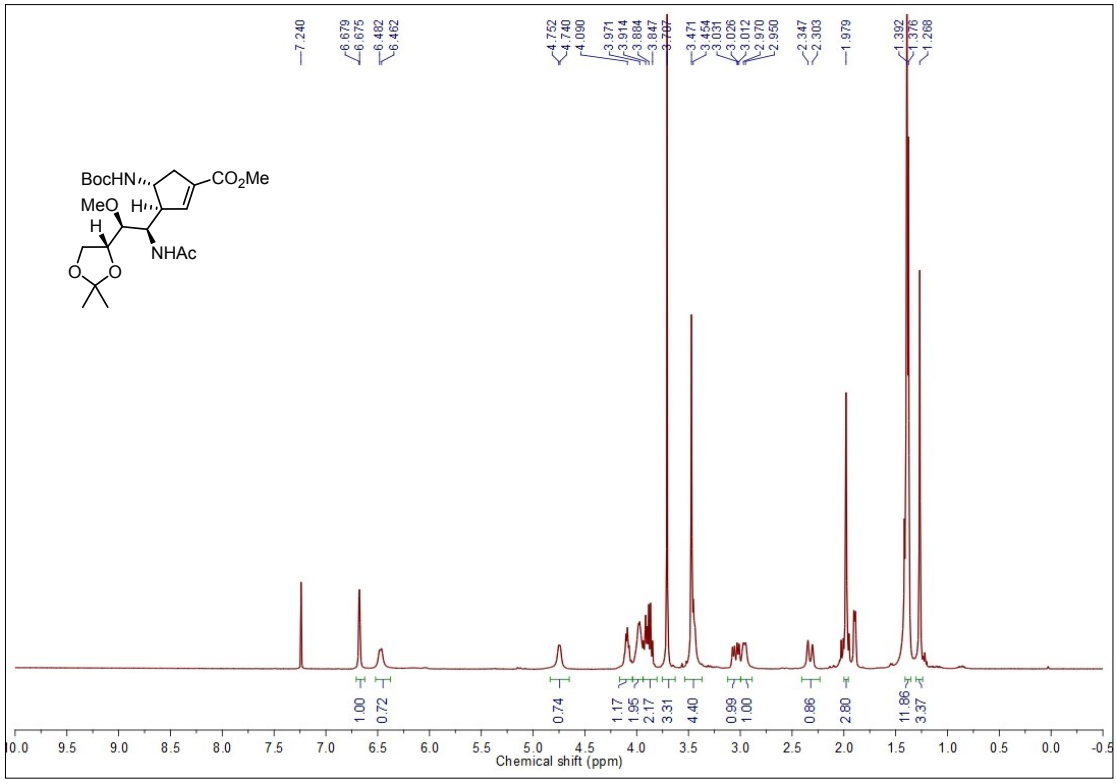
^{13}C NMR spectrum of compound **23a** (125 MHz, in $CDCl_3$)



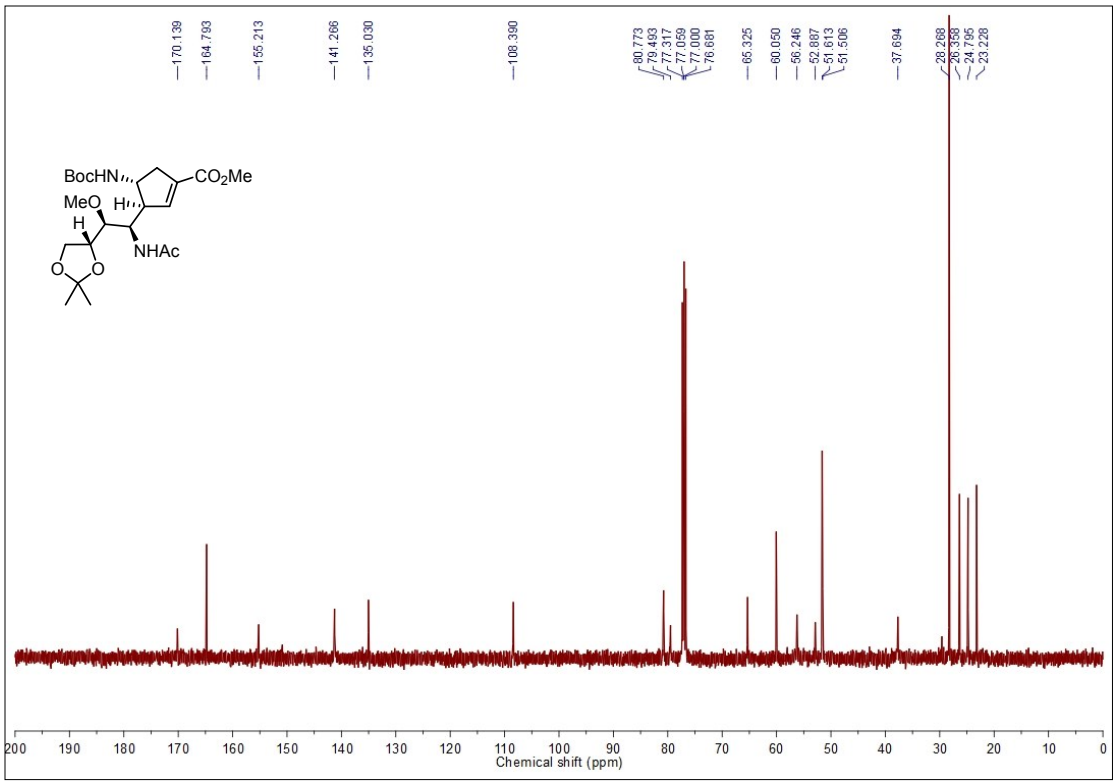
^{1}H NMR spectrum of compound **23b** (400 MHz, in $CDCl_3$)



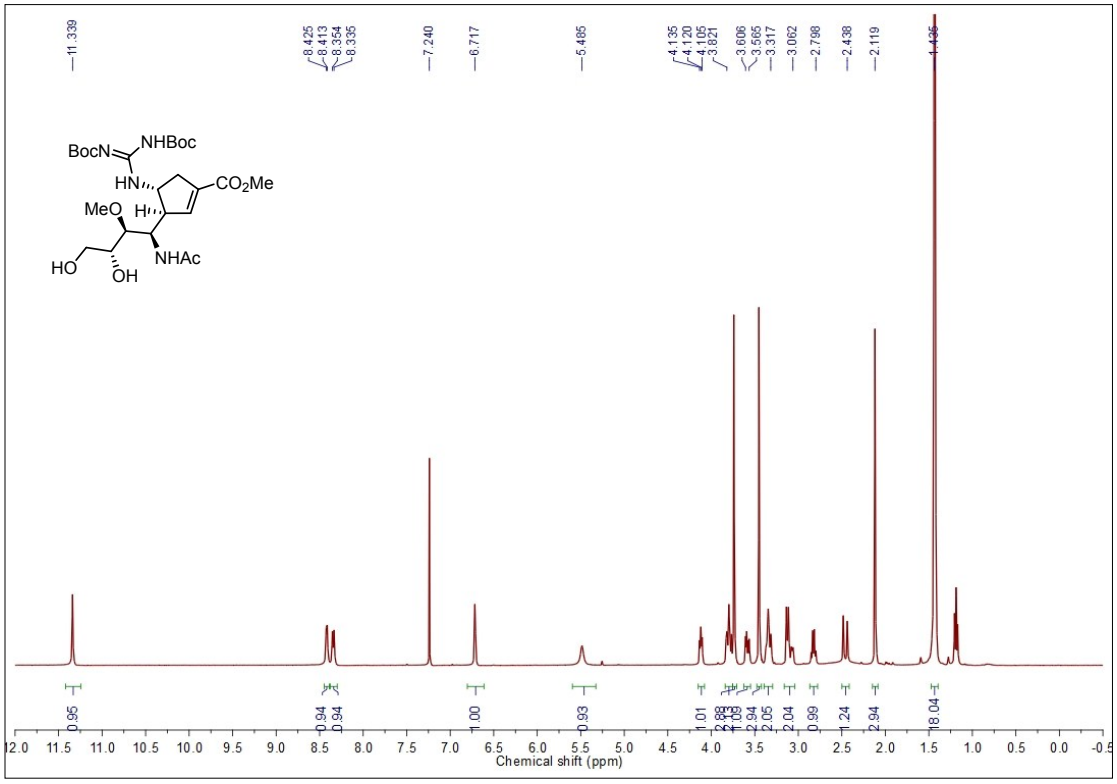
^{13}C NMR spectrum of compound **23b** (100 MHz, in $CDCl_3$)



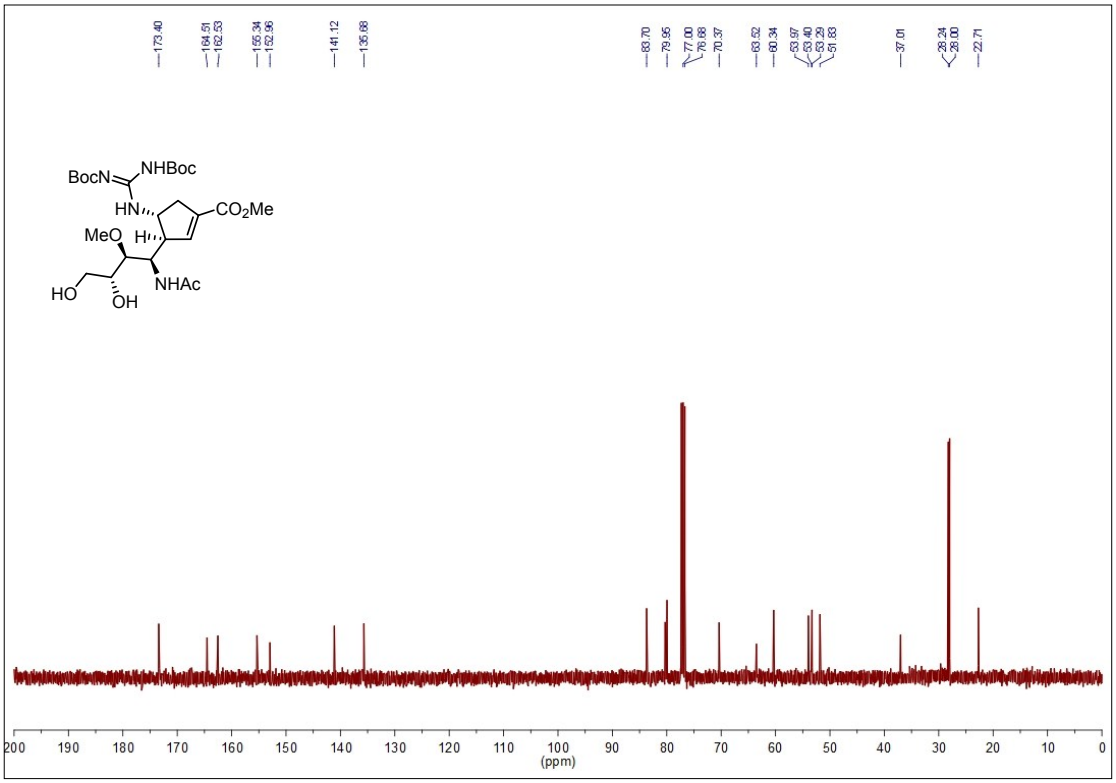
^{1}H NMR spectrum of compound **25** (400 MHz, in $CDCl_3$)



^{13}C NMR spectrum of compound **25** (100 MHz, in $CDCl_3$)



^{1}H NMR spectrum of compound **26** (400 MHz, in $CDCl_3$)



^{13}C NMR spectrum of compound **26** (100 MHz, in $CDCl_3$)