Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

D-Glucose Based Synthesis of Proline-Serine C-C Linked Central and Right Hand Core of Kaitocephalin-a Glutamate Receptor Antagonist.

Pramod R. Markad , Rajendra S. Rohokale, Nitin J. Pawar and Dilip D. Dhavale*

Department of chemistry, Garware Research Centre, Savitribai Phule Pune University (Formerly University of Pune), Pune-411007, India
ddd@chem.unipune.ac.in

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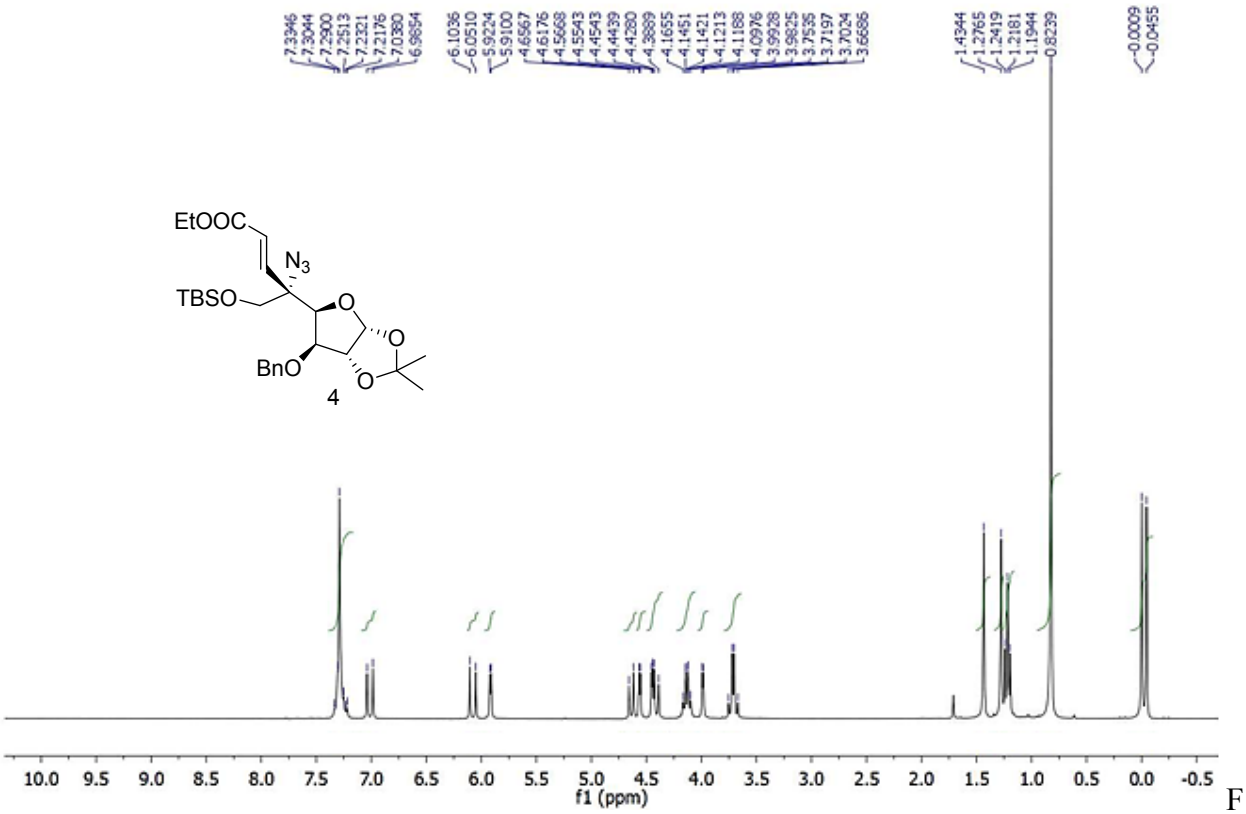

Figure 1: ^{1}H NMR of compound **4** (300 MHz, $CDCl_3$)

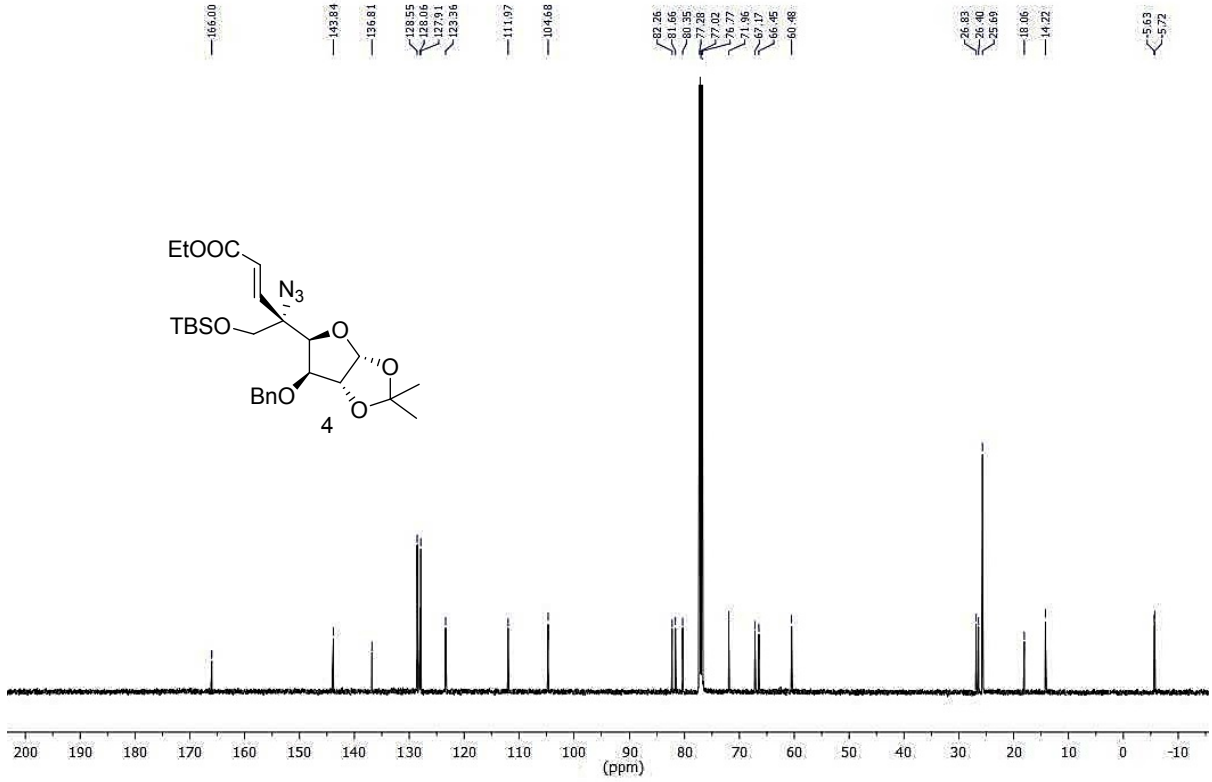

Figure 2: ^{13}C NMR of compound **4** (125 MHz, $CDCl_3$)

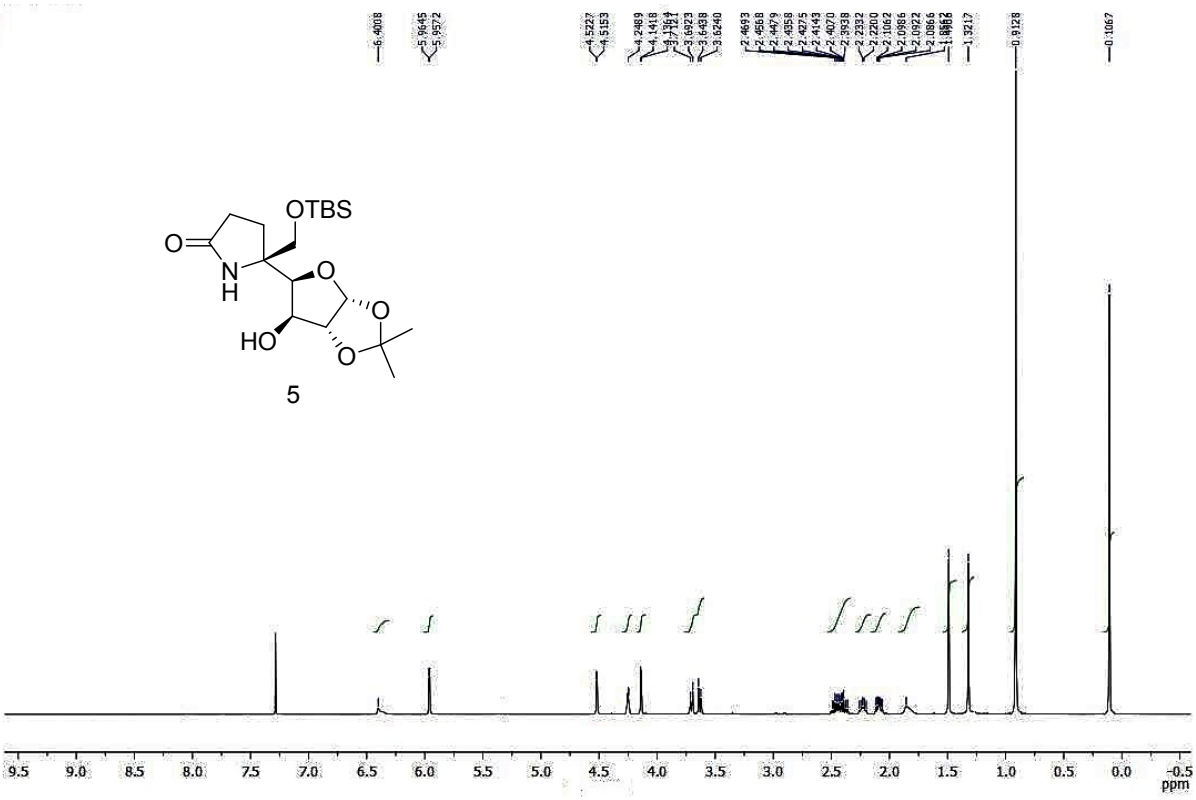

Figure 3: ^{1}H NMR of compound **5** (500 MHz, $CDCl_3$)

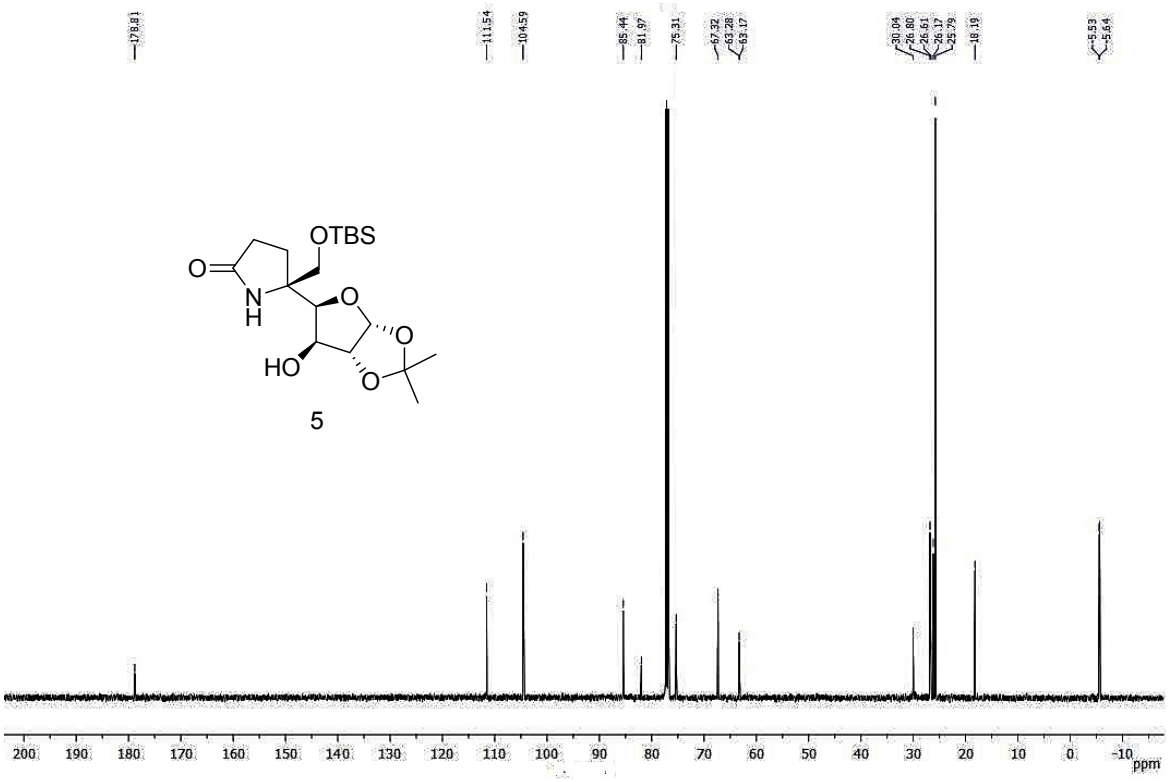

Figure 4: ^{13}C NMR of compound **5** (125 MHz, $CDCl_3$)

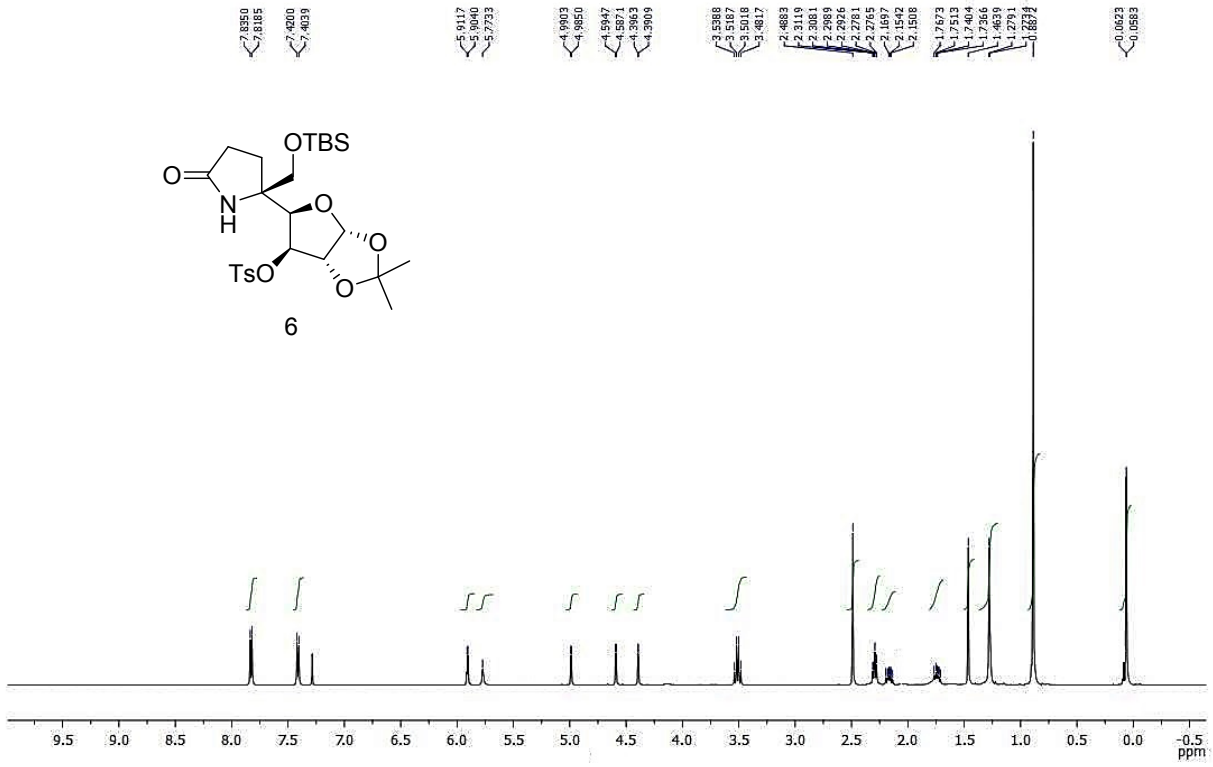

Figure 5: ^{1}H NMR of compound **6** (500 MHz, $CDCl_3$)

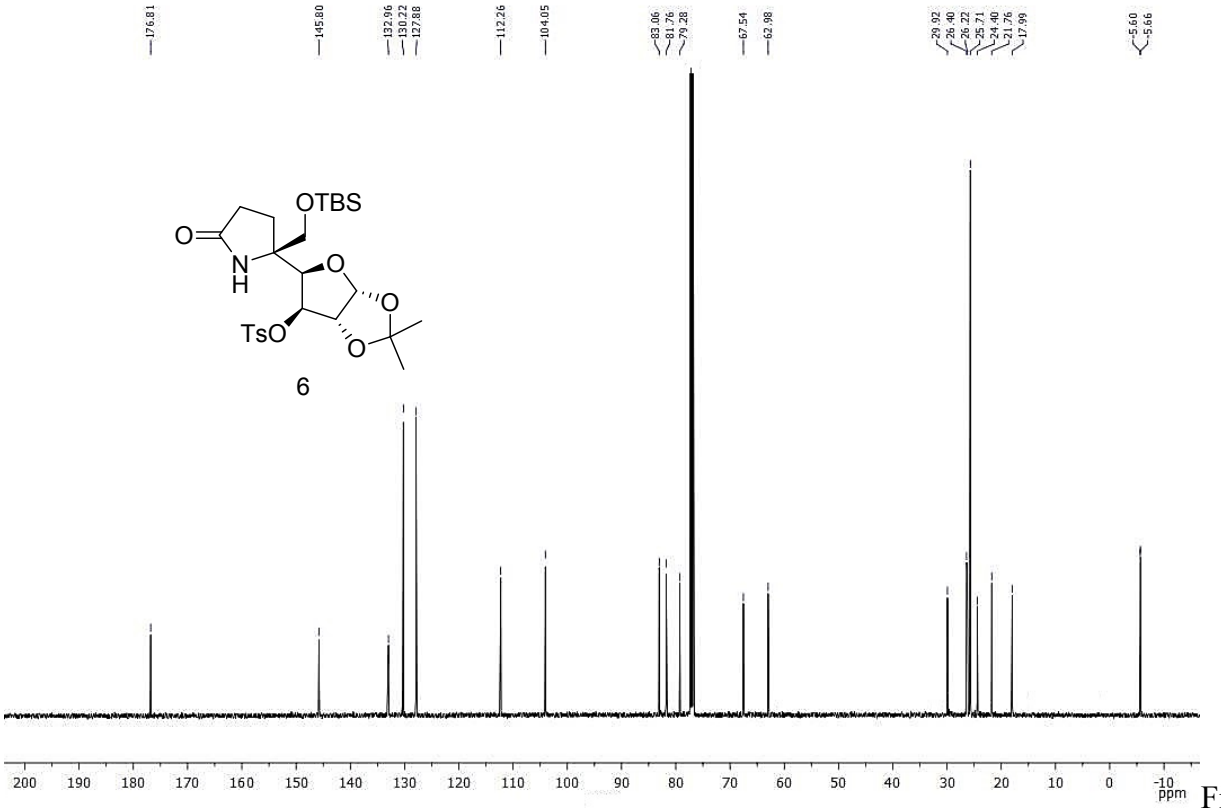

Figure 6: ^{13}C NMR of compound **6** (125 MHz, $CDCl_3$)

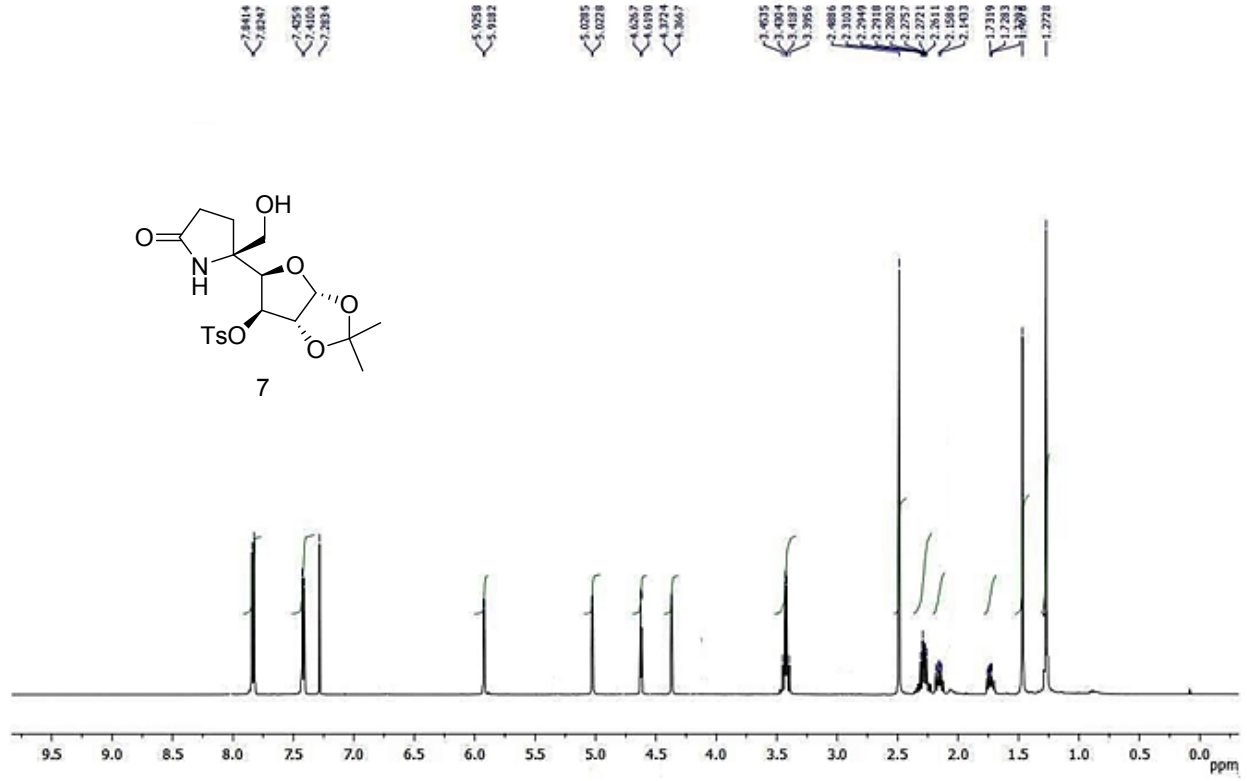

Figure 7: ^{1}H NMR of compound **7** (500 MHz, $CDCl_3$)

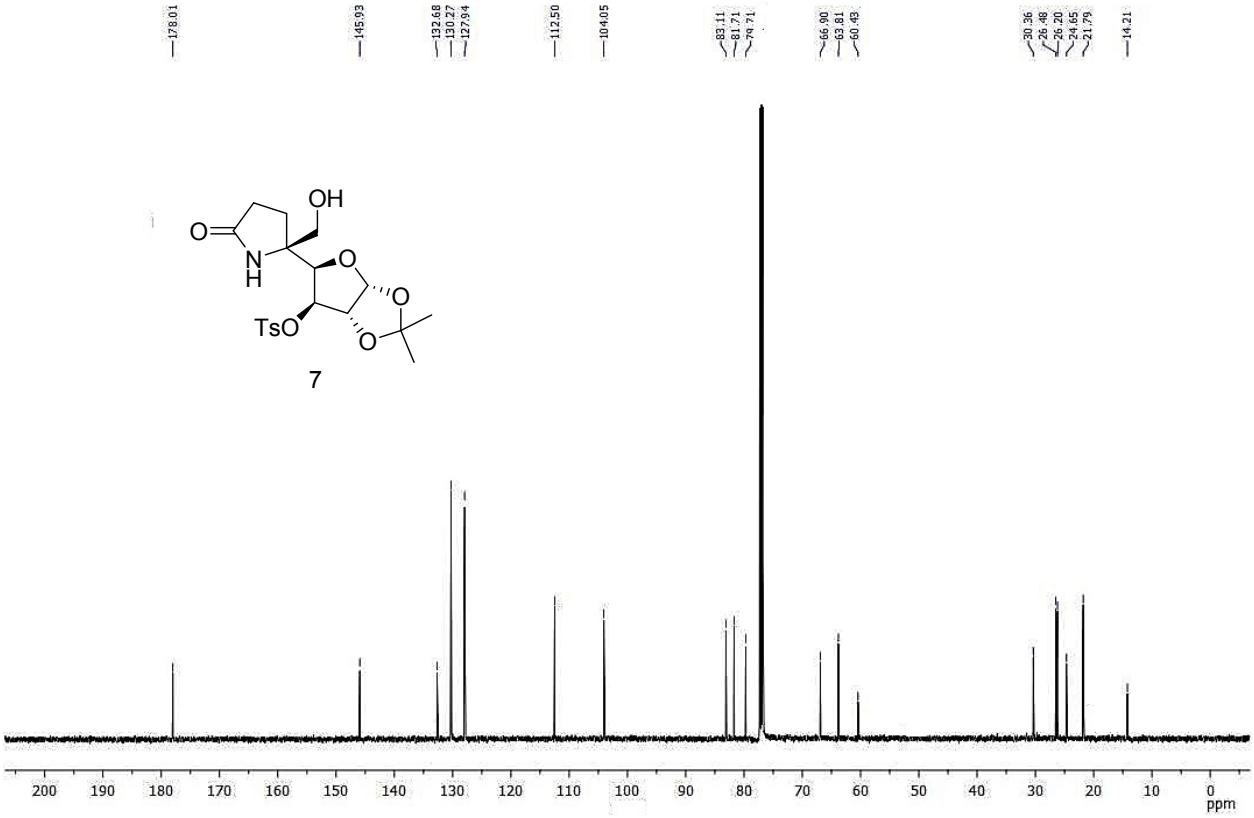

Figure 8: ^{13}C NMR of compound **7** (125 MHz, $CDCl_3$)

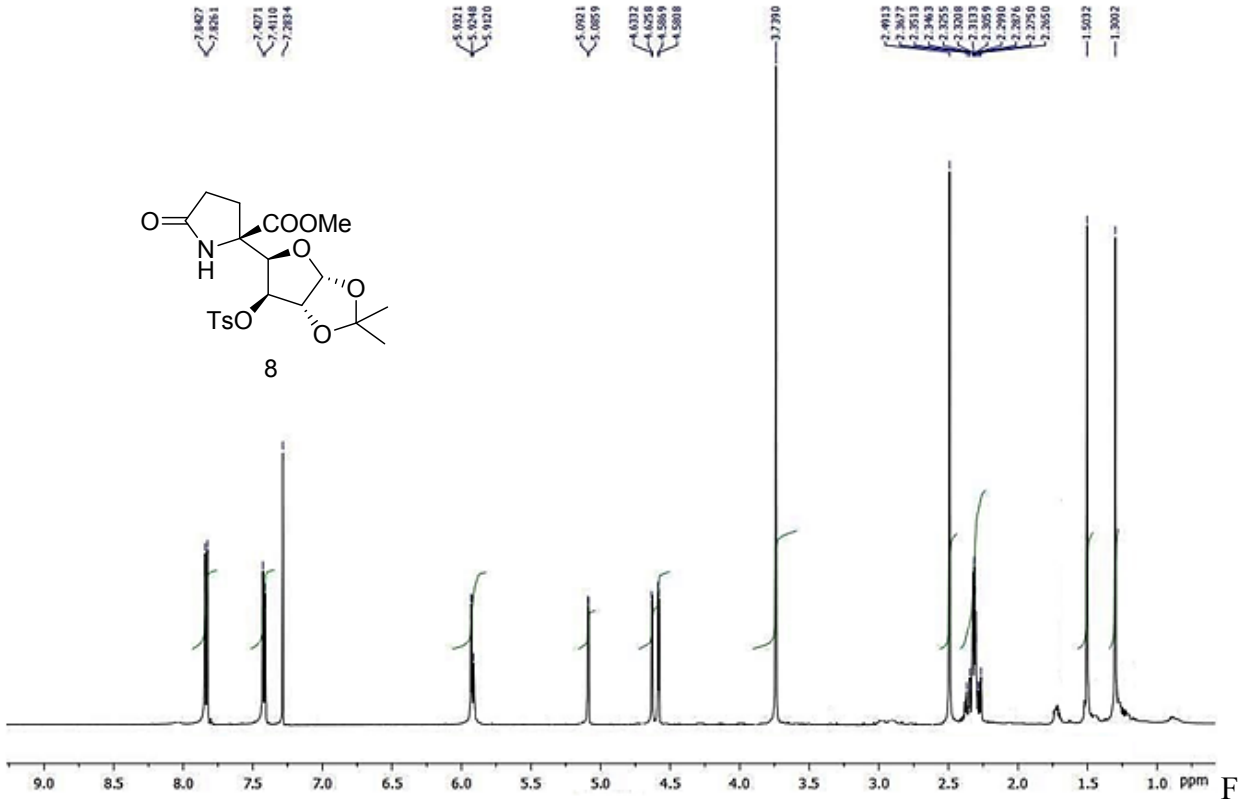

Figure 9: ^{1}H NMR of compound **8** (500 MHz, $CDCl_3$)

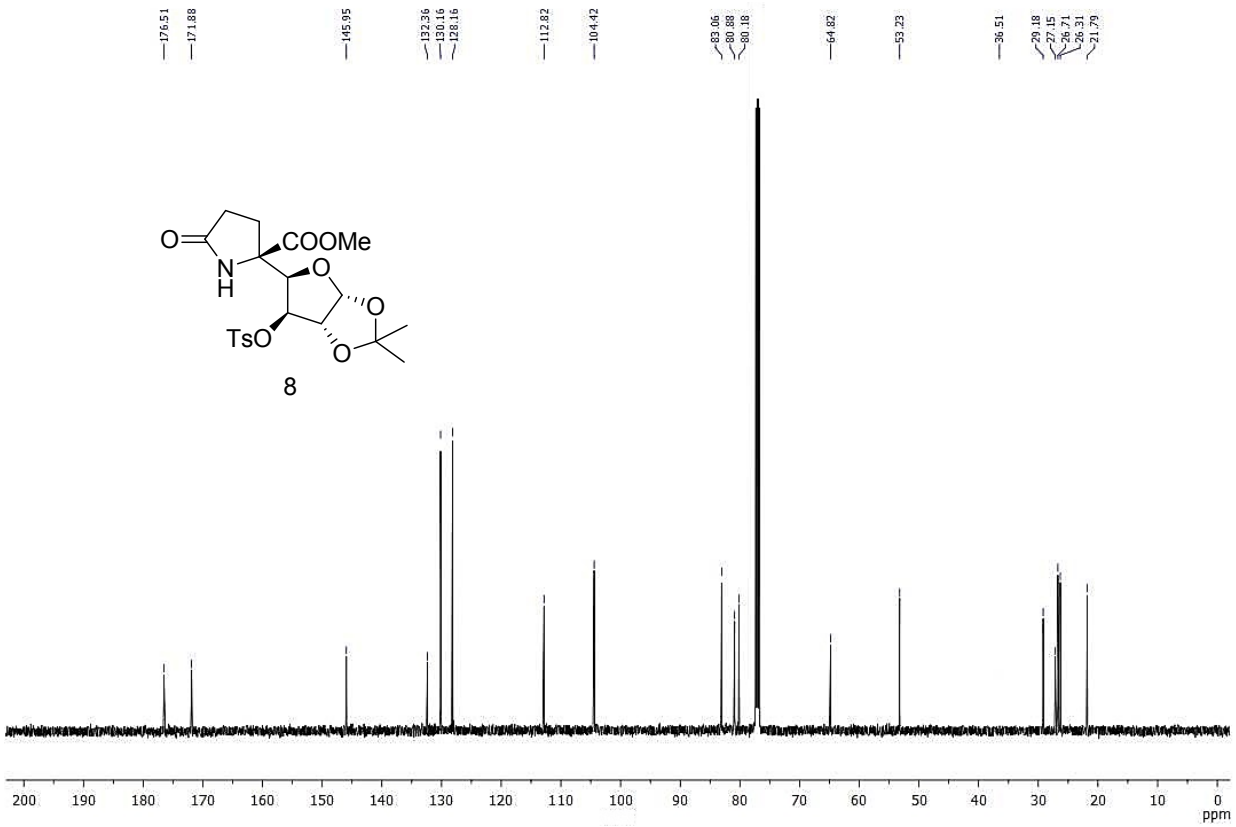

Figure 10: ^{13}C NMR of compound **8** (125 MHz, $CDCl_3$)

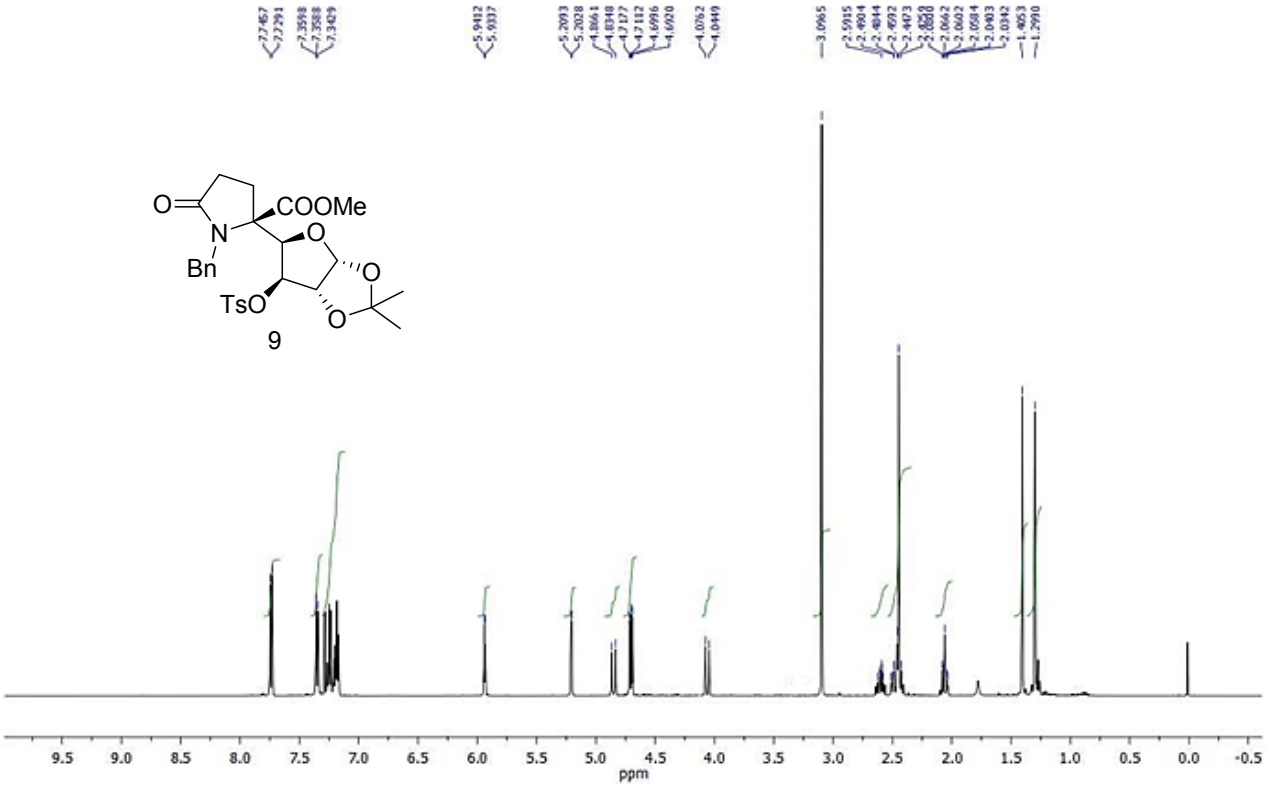

Figure 11: ^{1}H NMR of compound **9** (500 MHz, $CDCl_3$)

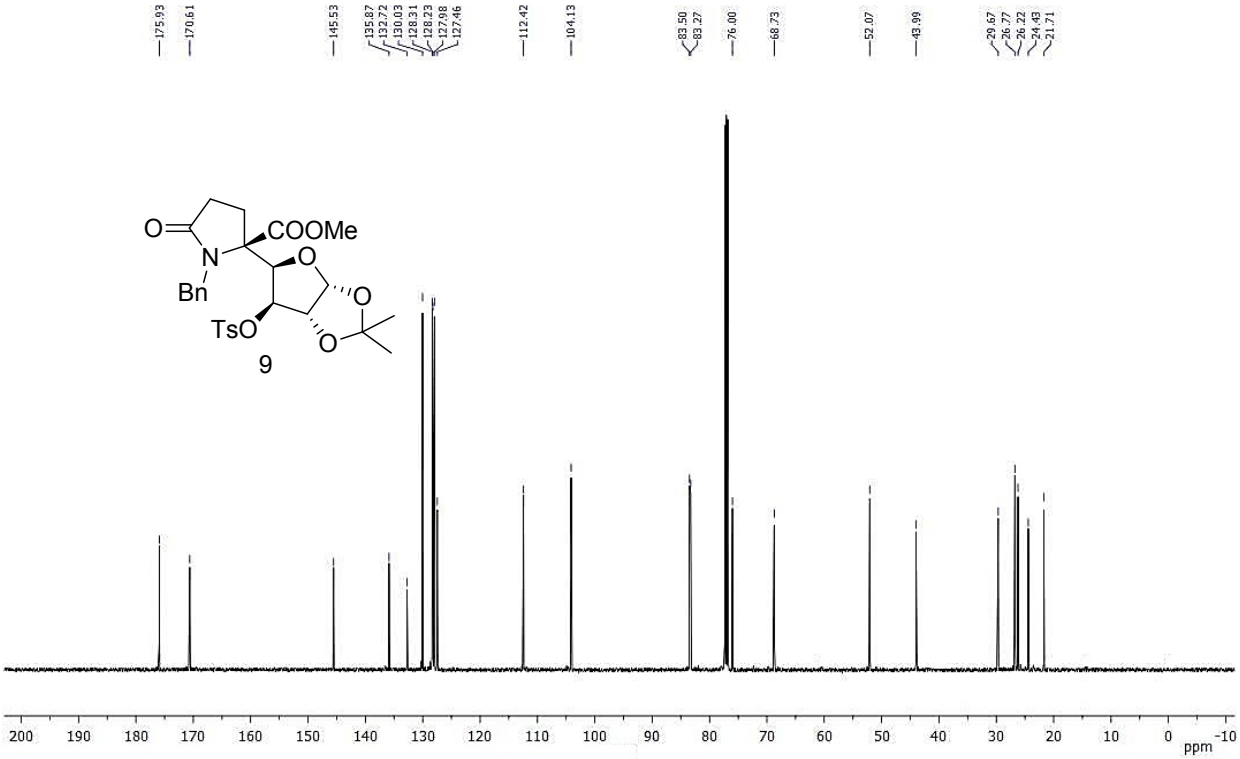

Figure 12: ^{13}C NMR of compound **9** (125 MHz, $CDCl_3$)

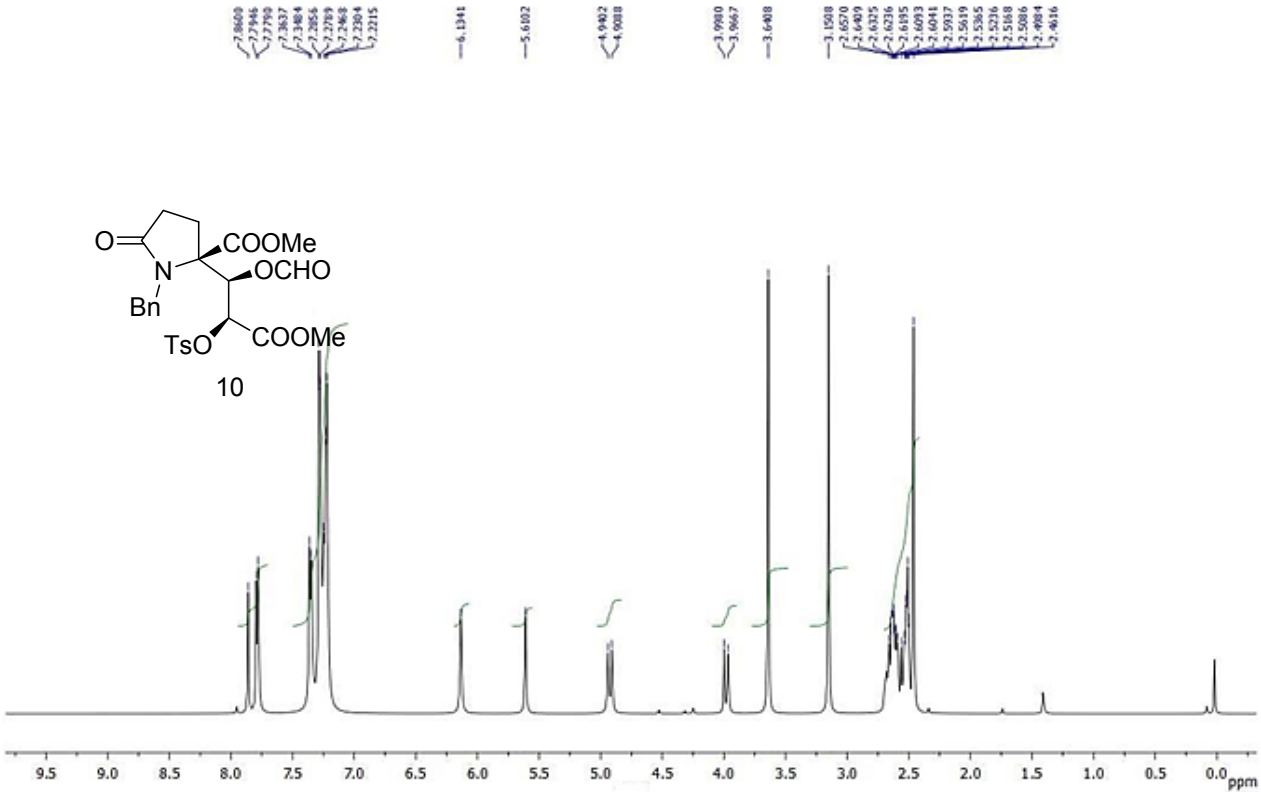

Figure 13: ^{1}H NMR of compound **10** (500 MHz, $CDCl_3$)

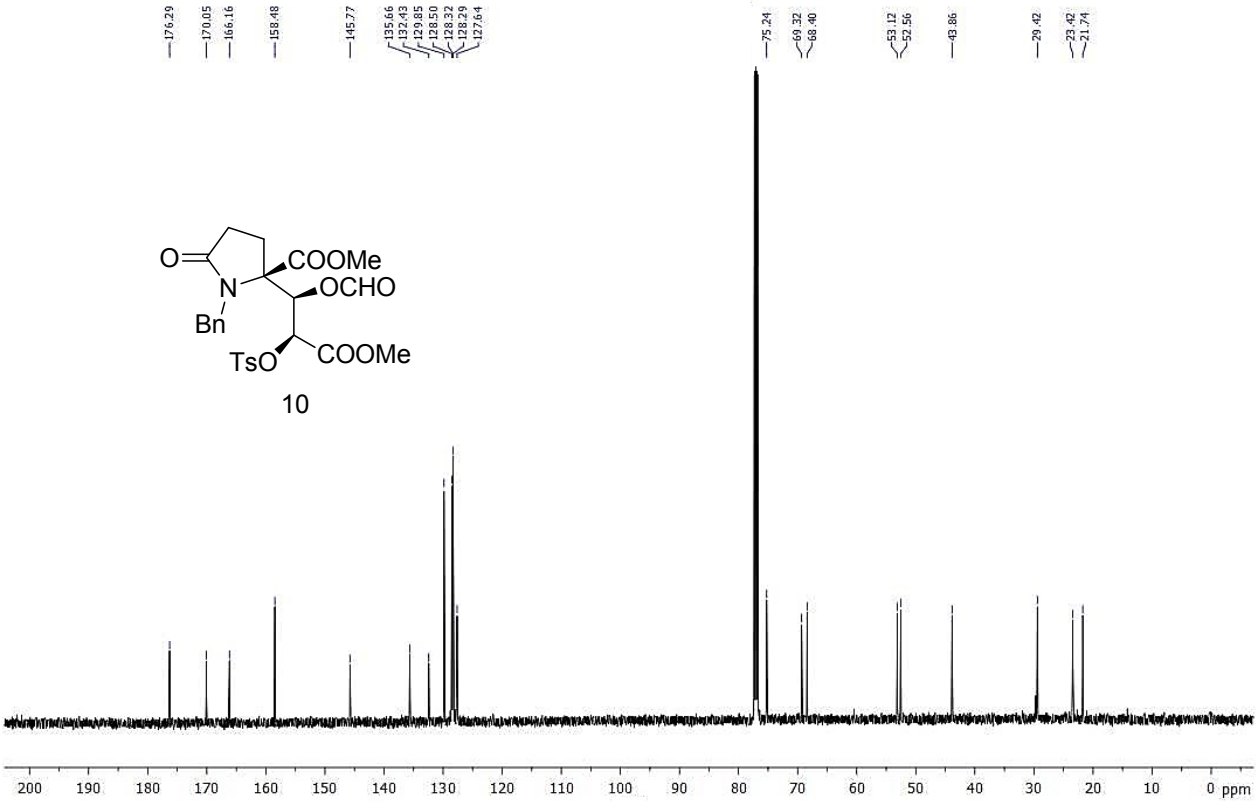

Figure 14: ^{13}C NMR of compound **10** (125 MHz, $CDCl_3$)

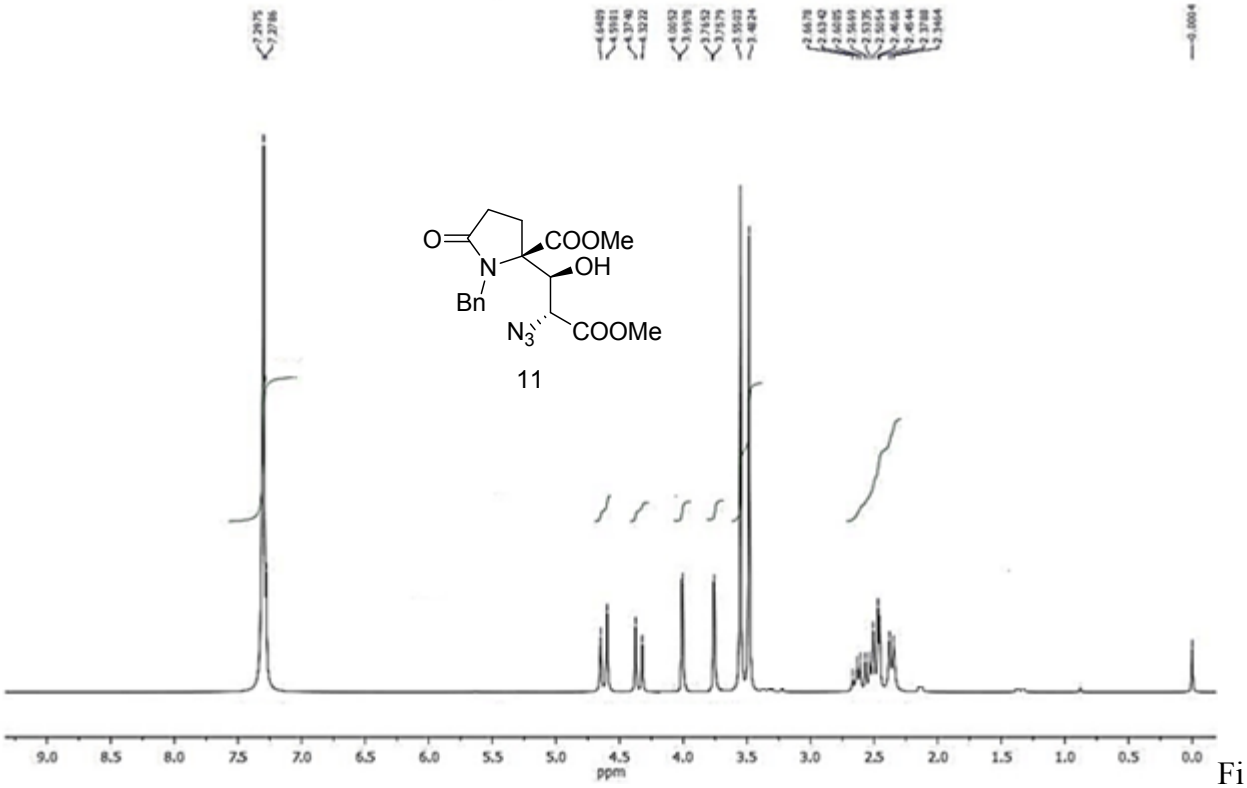

Figure 15: ^{1}H NMR of compound **11** (500 MHz, $CDCl_3$)

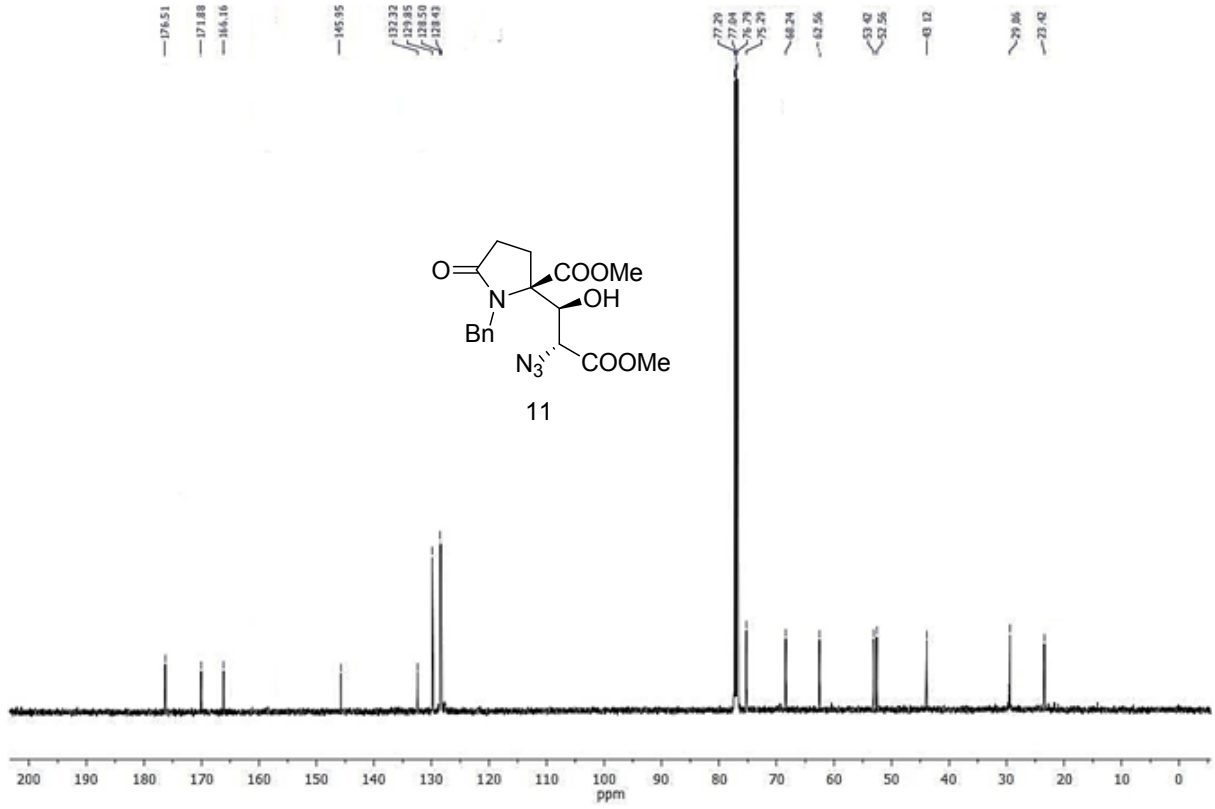

Figure 16: ^{13}C NMR of compound **11** (125 MHz, $CDCl_3$)

Figure 17: ORTEP diagram of compound **8**

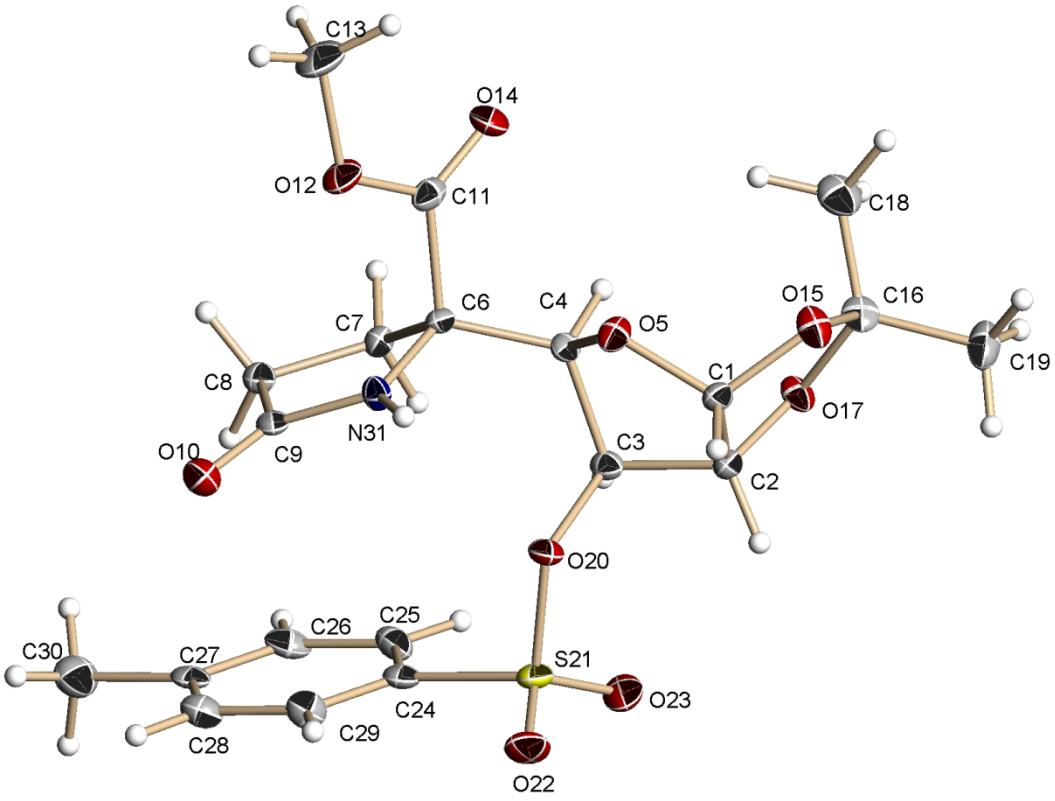

Table 1. Crystal data and structure refinement for mo_MPR_K_ESTER_0m (**8**).

Identification code	mo_mpr_k_ester_0m	
Empirical formula	C20 H25 N O9 S	
Formula weight	455.47	
Temperature	0(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 8.5776(3) Å	α= 90°.
	b = 6.3520(2) Å	β= 91.3640(9)°.
	c = 19.1584(8) Å	γ = 90°.
Volume	1043.55(6) $Å^3$	
Z	2	
Density (calculated)	1.450 g/cc^3	
Absorption coefficient	0.209 mm^{-1}	
F(000)	480	
Crystal size	0.46 x 0.24 x 0.09 mm^3	
Theta range for data collection	3.15 to 28.31°.	
Index ranges	-11<=h<=11, -8<=k<=8, -25<=l<=25	
Reflections collected	27491	
Independent reflections	5176 [R(int) = 0.0971]	
Completeness to theta = 28.31°	99.5 %	
Max. and min. transmission	0.9821 and 0.9099	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5176 / 1 / 285	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0574, wR2 = 0.0858	
R indices (all data)	R1 = 0.1095, wR2 = 0.0992	
Absolute structure parameter	0.14(9)	
Extinction coefficient	0.0166(16)	
Largest diff. peak and hole	0.334 and -0.348 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_MPR_K_ESTER_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(21)	-7(1)	628(1)	6970(1)	22(1)
O(5)	3228(2)	1249(3)	8782(1)	17(1)
O(10)	3636(2)	6226(3)	6690(1)	23(1)
O(12)	6536(2)	4385(3)	8158(1)	24(1)
O(14)	6878(2)	1030(3)	8501(1)	26(1)
O(15)	2267(2)	-1065(3)	9623(1)	20(1)
O(17)	2228(2)	-3340(3)	8694(1)	18(1)
O(20)	1251(2)	1090(3)	7563(1)	17(1)
O(22)	-1203(2)	2127(4)	7086(1)	32(1)
O(23)	-348(3)	-1573(3)	6965(1)	30(1)
N(31)	3825(3)	3799(3)	7565(1)	15(1)
C(1)	1920(3)	131(4)	9030(1)	16(1)
C(2)	1467(3)	-1465(4)	8465(1)	16(1)
C(3)	2237(3)	-617(5)	7823(1)	15(1)
C(4)	3741(3)	299(5)	8140(1)	15(1)
C(6)	4673(3)	1897(4)	7749(1)	14(1)
C(7)	5167(3)	1060(4)	7023(1)	16(1)
C(8)	5199(3)	3042(4)	6574(2)	17(1)
C(9)	4139(3)	4564(5)	6930(2)	16(1)
C(11)	6149(3)	2362(5)	8189(2)	18(1)
C(13)	7956(4)	4976(6)	8529(2)	38(1)
C(16)	2616(3)	-3204(5)	9433(2)	19(1)
C(18)	4327(3)	-3653(5)	9536(2)	27(1)
C(19)	1594(4)	-4623(5)	9844(2)	27(1)
C(24)	919(3)	1318(5)	6196(2)	20(1)
C(25)	1787(3)	-191(5)	5850(2)	21(1)
C(26)	2519(3)	381(5)	5240(2)	22(1)
C(27)	2382(3)	2413(5)	4972(2)	20(1)
C(28)	1493(3)	3870(5)	5329(2)	23(1)
C(29)	774(3)	3336(5)	5943(2)	21(1)
C(30)	3189(4)	3016(6)	4312(2)	30(1)

Table 3. Bond lengths [Å] and angles [°] for mo_MPR_K_ESTER_0m.

S(21)-O(22)	1.421(2)
S(21)-O(23)	1.428(2)
S(21)-O(20)	1.5766(18)
S(21)-C(24)	1.755(3)
O(5)-C(1)	1.419(3)
O(5)-C(4)	1.447(3)
O(10)-C(9)	1.225(3)
O(12)-C(11)	1.329(3)
O(12)-C(13)	1.445(3)
O(14)-C(11)	1.203(3)
O(15)-C(1)	1.394(3)
O(15)-C(16)	1.440(3)
O(17)-C(2)	1.422(3)
O(17)-C(16)	1.450(3)
O(20)-C(3)	1.455(3)
N(31)-C(9)	1.344(4)
N(31)-C(6)	1.449(3)
N(31)-H(31)	0.8800
C(1)-C(2)	1.525(4)
C(1)-H(1)	1.0000
C(2)-C(3)	1.510(4)
C(2)-H(2)	1.0000
C(3)-C(4)	1.529(4)
C(3)-H(3)	1.0000
C(4)-C(6)	1.504(4)
C(4)-H(4)	1.0000
C(6)-C(11)	1.533(4)
C(6)-C(7)	1.556(4)
C(7)-C(8)	1.525(4)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.502(4)
C(8)-H(8A)	0.9900

C(8)-H(8B)	0.9900
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(16)-C(19)	1.495(4)
C(16)-C(18)	1.503(4)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(24)-C(29)	1.375(4)
C(24)-C(25)	1.392(4)
C(25)-C(26)	1.387(4)
C(25)-H(25)	0.9500
C(26)-C(27)	1.394(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.389(4)
C(27)-C(30)	1.505(4)
C(28)-C(29)	1.384(4)
C(28)-H(28)	0.9500
C(29)-H(29)	0.9500
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800

O(22)-S(21)-O(23)	120.59(14)
O(22)-S(21)-O(20)	104.28(13)
O(23)-S(21)-O(20)	108.84(12)
O(22)-S(21)-C(24)	107.93(14)
O(23)-S(21)-C(24)	109.65(14)
O(20)-S(21)-C(24)	104.28(11)
C(1)-O(5)-C(4)	109.5(2)
C(11)-O(12)-C(13)	116.0(2)
C(1)-O(15)-C(16)	110.4(2)

C(2)-O(17)-C(16)	110.2(2)
C(3)-O(20)-S(21)	119.32(17)
C(9)-N(31)-C(6)	114.3(2)
C(9)-N(31)-H(31)	122.9
C(6)-N(31)-H(31)	122.9
O(15)-C(1)-O(5)	113.0(2)
O(15)-C(1)-C(2)	105.2(2)
O(5)-C(1)-C(2)	106.6(2)
O(15)-C(1)-H(1)	110.6
O(5)-C(1)-H(1)	110.6
C(2)-C(1)-H(1)	110.6
O(17)-C(2)-C(3)	110.1(2)
O(17)-C(2)-C(1)	103.3(2)
C(3)-C(2)-C(1)	103.4(2)
O(17)-C(2)-H(2)	113.0
C(3)-C(2)-H(2)	113.0
C(1)-C(2)-H(2)	113.0
O(20)-C(3)-C(2)	106.4(2)
O(20)-C(3)-C(4)	109.3(2)
C(2)-C(3)-C(4)	101.1(2)
O(20)-C(3)-H(3)	113.1
C(2)-C(3)-H(3)	113.1
C(4)-C(3)-H(3)	113.1
O(5)-C(4)-C(6)	108.6(2)
O(5)-C(4)-C(3)	103.1(2)
C(6)-C(4)-C(3)	120.8(2)
O(5)-C(4)-H(4)	107.9
C(6)-C(4)-H(4)	107.9
C(3)-C(4)-H(4)	107.9
N(31)-C(6)-C(4)	114.5(2)
N(31)-C(6)-C(11)	112.1(2)
C(4)-C(6)-C(11)	107.3(2)
N(31)-C(6)-C(7)	102.3(2)
C(4)-C(6)-C(7)	112.0(2)
C(11)-C(6)-C(7)	108.6(2)
C(8)-C(7)-C(6)	103.3(2)

C(8)-C(7)-H(7A)	111.1
C(6)-C(7)-H(7A)	111.1
C(8)-C(7)-H(7B)	111.1
C(6)-C(7)-H(7B)	111.1
H(7A)-C(7)-H(7B)	109.1
C(9)-C(8)-C(7)	104.9(2)
C(9)-C(8)-H(8A)	110.8
C(7)-C(8)-H(8A)	110.8
C(9)-C(8)-H(8B)	110.8
C(7)-C(8)-H(8B)	110.8
H(8A)-C(8)-H(8B)	108.9
O(10)-C(9)-N(31)	125.0(3)
O(10)-C(9)-C(8)	126.6(3)
N(31)-C(9)-C(8)	108.3(2)
O(14)-C(11)-O(12)	125.1(3)
O(14)-C(11)-C(6)	123.4(3)
O(12)-C(11)-C(6)	111.4(2)
O(12)-C(13)-H(13A)	109.5
O(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
O(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
O(15)-C(16)-O(17)	105.0(2)
O(15)-C(16)-C(19)	107.9(2)
O(17)-C(16)-C(19)	110.8(2)
O(15)-C(16)-C(18)	110.8(2)
O(17)-C(16)-C(18)	108.5(2)
C(19)-C(16)-C(18)	113.6(3)
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5

C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(29)-C(24)-C(25)	121.3(3)
C(29)-C(24)-S(21)	119.4(2)
C(25)-C(24)-S(21)	119.2(2)
C(26)-C(25)-C(24)	118.6(3)
C(26)-C(25)-H(25)	120.7
C(24)-C(25)-H(25)	120.7
C(25)-C(26)-C(27)	121.2(3)
C(25)-C(26)-H(26)	119.4
C(27)-C(26)-H(26)	119.4
C(28)-C(27)-C(26)	118.5(3)
C(28)-C(27)-C(30)	120.8(3)
C(26)-C(27)-C(30)	120.6(3)
C(29)-C(28)-C(27)	121.1(3)
C(29)-C(28)-H(28)	119.4
C(27)-C(28)-H(28)	119.4
C(24)-C(29)-C(28)	119.3(3)
C(24)-C(29)-H(29)	120.4
C(28)-C(29)-H(29)	120.4
C(27)-C(30)-H(30A)	109.5
C(27)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(27)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_MPR_K_ESTER_0m. 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}
S(21)	13(1)	34(1)	20(1)	6(1)	-6(1)	-6(1)
O(5)	19(1)	21(1)	12(1)	-4(1)	1(1)	-7(1)
O(10)	23(1)	22(1)	23(1)	3(1)	-2(1)	2(1)
O(12)	20(1)	26(1)	25(1)	-2(1)	-4(1)	-11(1)
O(14)	22(1)	35(1)	22(1)	9(1)	-9(1)	-4(1)
O(15)	30(1)	15(1)	13(1)	-2(1)	1(1)	-1(1)
O(17)	26(1)	16(1)	10(1)	-1(1)	-4(1)	-1(1)
O(20)	15(1)	20(1)	16(1)	2(1)	-6(1)	-1(1)
O(22)	12(1)	56(2)	28(1)	10(1)	2(1)	6(1)
O(23)	31(1)	33(1)	27(1)	5(1)	-12(1)	-19(1)
N(31)	17(1)	12(1)	15(1)	2(1)	2(1)	2(1)
C(1)	11(1)	22(2)	16(2)	3(1)	1(1)	-1(1)
C(2)	13(1)	18(2)	16(2)	3(1)	0(1)	-2(1)
C(3)	15(1)	14(2)	17(2)	0(1)	-3(1)	0(1)
C(4)	15(1)	21(2)	9(1)	1(1)	0(1)	-3(1)
C(6)	10(1)	18(2)	14(2)	2(1)	-1(1)	-2(1)
C(7)	14(1)	16(2)	17(2)	2(1)	1(1)	-2(1)
C(8)	15(2)	21(2)	15(2)	1(1)	0(1)	-1(1)
C(9)	13(1)	19(2)	14(2)	0(1)	-6(1)	-5(1)
C(11)	15(2)	28(2)	12(2)	-3(1)	2(1)	-6(1)
C(13)	26(2)	50(3)	37(2)	0(2)	-11(2)	-20(2)
C(16)	26(2)	20(2)	11(2)	-6(1)	-3(1)	-5(1)
C(18)	33(2)	29(2)	18(2)	-3(1)	-4(1)	-1(2)
C(19)	37(2)	25(2)	19(2)	1(2)	3(1)	-13(2)
C(24)	14(1)	28(2)	17(2)	3(1)	-7(1)	-3(1)
C(25)	25(2)	19(2)	19(2)	3(1)	-7(1)	0(1)
C(26)	21(2)	28(2)	16(2)	-4(2)	-7(1)	5(1)
C(27)	15(2)	30(2)	15(2)	1(1)	-8(1)	-3(1)
C(28)	22(2)	24(2)	22(2)	1(1)	-5(1)	3(1)
C(29)	22(2)	22(2)	20(2)	-2(1)	1(1)	3(1)
C(30)	30(2)	39(2)	22(2)	2(2)	-1(2)	0(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_MPR_K_ESTER_0m.

	x	y	z	U(eq)
H(31)	3162	4402	7846	18
H(1)	1035	1114	9117	20
H(2)	313	-1636	8403	19
H(3)	2427	-1724	7463	18
H(4)	4448	-900	8266	18
H(7A)	6208	389	7053	19
H(7B)	4401	30	6834	19
H(8A)	6271	3614	6553	20
H(8B)	4814	2740	6093	20
H(13A)	7895	4538	9018	57
H(13B)	8088	6507	8506	57
H(13C)	8846	4285	8314	57
H(18A)	4933	-2566	9300	40
H(18B)	4568	-5034	9337	40
H(18C)	4596	-3651	10036	40
H(19A)	1730	-4310	10343	40
H(19B)	1879	-6092	9758	40
H(19C)	502	-4397	9701	40
H(25)	1876	-1584	6027	25
H(26)	3124	-630	5002	26
H(28)	1377	5255	5148	27
H(29)	187	4354	6188	26
H(30A)	2579	2508	3907	45
H(30B)	4230	2381	4311	45
H(30C)	3283	4552	4288	45

Table 6. Torsion angles [°] for mo_MPR_K_ESTER_0m.

O(22)-S(21)-O(20)-C(3)	151.27(19)
O(23)-S(21)-O(20)-C(3)	21.4(2)
C(24)-S(21)-O(20)-C(3)	-95.6(2)
C(16)-O(15)-C(1)-O(5)	-95.4(3)
C(16)-O(15)-C(1)-C(2)	20.5(3)
C(4)-O(5)-C(1)-O(15)	108.3(2)
C(4)-O(5)-C(1)-C(2)	-6.7(3)
C(16)-O(17)-C(2)-C(3)	129.6(2)
C(16)-O(17)-C(2)-C(1)	19.7(3)
O(15)-C(1)-C(2)-O(17)	-24.3(3)
O(5)-C(1)-C(2)-O(17)	95.9(2)
O(15)-C(1)-C(2)-C(3)	-139.1(2)
O(5)-C(1)-C(2)-C(3)	-18.9(3)
S(21)-O(20)-C(3)-C(2)	-95.4(2)
S(21)-O(20)-C(3)-C(4)	156.25(17)
O(17)-C(2)-C(3)-O(20)	171.4(2)
C(1)-C(2)-C(3)-O(20)	-78.7(2)
O(17)-C(2)-C(3)-C(4)	-74.5(3)
C(1)-C(2)-C(3)-C(4)	35.4(3)
C(1)-O(5)-C(4)-C(6)	158.7(2)
C(1)-O(5)-C(4)-C(3)	29.4(3)
O(20)-C(3)-C(4)-O(5)	72.2(2)
C(2)-C(3)-C(4)-O(5)	-39.7(3)
O(20)-C(3)-C(4)-C(6)	-49.1(3)
C(2)-C(3)-C(4)-C(6)	-161.0(2)
C(9)-N(31)-C(6)-C(4)	-141.2(2)
C(9)-N(31)-C(6)-C(11)	96.4(3)
C(9)-N(31)-C(6)-C(7)	-19.8(3)
O(5)-C(4)-C(6)-N(31)	-59.8(3)
C(3)-C(4)-C(6)-N(31)	58.8(3)
O(5)-C(4)-C(6)-C(11)	65.2(3)
C(3)-C(4)-C(6)-C(11)	-176.2(2)
O(5)-C(4)-C(6)-C(7)	-175.71(19)
C(3)-C(4)-C(6)-C(7)	-57.1(3)

N(31)-C(6)-C(7)-C(8)	25.4(2)
C(4)-C(6)-C(7)-C(8)	148.5(2)
C(11)-C(6)-C(7)-C(8)	-93.2(3)
C(6)-C(7)-C(8)-C(9)	-23.1(3)
C(6)-N(31)-C(9)-O(10)	-174.8(2)
C(6)-N(31)-C(9)-C(8)	5.2(3)
C(7)-C(8)-C(9)-O(10)	-167.8(3)
C(7)-C(8)-C(9)-N(31)	12.3(3)
C(13)-O(12)-C(11)-O(14)	0.5(4)
C(13)-O(12)-C(11)-C(6)	-177.2(2)
N(31)-C(6)-C(11)-O(14)	166.5(3)
C(4)-C(6)-C(11)-O(14)	40.0(4)
C(7)-C(6)-C(11)-O(14)	-81.2(3)
N(31)-C(6)-C(11)-O(12)	-15.8(3)
C(4)-C(6)-C(11)-O(12)	-142.3(2)
C(7)-C(6)-C(11)-O(12)	96.5(3)
C(1)-O(15)-C(16)-O(17)	-8.6(3)
C(1)-O(15)-C(16)-C(19)	-126.8(2)
C(1)-O(15)-C(16)-C(18)	108.3(3)
C(2)-O(17)-C(16)-O(15)	-8.0(3)
C(2)-O(17)-C(16)-C(19)	108.2(3)
C(2)-O(17)-C(16)-C(18)	-126.5(2)
O(22)-S(21)-C(24)-C(29)	19.6(3)
O(23)-S(21)-C(24)-C(29)	152.7(2)
O(20)-S(21)-C(24)-C(29)	-90.9(2)
O(22)-S(21)-C(24)-C(25)	-160.4(2)
O(23)-S(21)-C(24)-C(25)	-27.3(3)
O(20)-S(21)-C(24)-C(25)	89.1(2)
C(29)-C(24)-C(25)-C(26)	0.3(4)
S(21)-C(24)-C(25)-C(26)	-179.7(2)
C(24)-C(25)-C(26)-C(27)	-0.7(4)
C(25)-C(26)-C(27)-C(28)	0.1(4)
C(25)-C(26)-C(27)-C(30)	179.7(3)
C(26)-C(27)-C(28)-C(29)	0.9(4)
C(30)-C(27)-C(28)-C(29)	-178.7(3)
C(25)-C(24)-C(29)-C(28)	0.7(4)

S(21)-C(24)-C(29)-C(28)	-179.3(2)
C(27)-C(28)-C(29)-C(24)	-1.3(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_MPR_K_ESTER_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(25)-H(25)...O(10)#1	0.95	2.40	3.189(4)	140.8
C(19)-H(19A)...O(14)#2	0.98	2.50	3.427(4)	157.5
C(13)-H(13A)...O(15)#3	0.98	2.64	3.611(4)	171.8
C(8)-H(8A)...O(22)#4	0.99	2.55	3.268(3)	128.9
C(7)-H(7B)...O(10)#1	0.99	2.52	3.394(3)	147.5
C(7)-H(7A)...O(22)#4	0.99	2.48	3.186(3)	128.0
C(3)-H(3)...O(10)#1	1.00	2.24	3.208(3)	161.3
N(31)-H(31)...O(17)#5	0.88	2.32	3.163(3)	159.1
C(25)-H(25)...O(10)#1	0.95	2.40	3.189(4)	140.8
C(19)-H(19A)...O(14)#2	0.98	2.50	3.427(4)	157.5
C(13)-H(13A)...O(15)#3	0.98	2.64	3.611(4)	171.8
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C(8)-H(8A)...O(22)#4	0.99	2.55	3.268(3)	128.9
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C(7)-H(7B)...O(10)#1	0.99	2.52	3.394(3)	147.5
N(31)-H(31)...O(17)#5	0.88	2.32	3.163(3)	159.1
C(3)-H(3)...O(10)#1	1.00	2.24	3.208(3)	161.3
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C(25)-H(25)...O(10)#1	0.95	2.40	3.189(4)	140.8

N(31)-H(31)...O(17)#5	0.88	2.32	3.163(3)	159.1
C(3)-H(3)...O(10)#1	1.00	2.24	3.208(3)	161.3
C(7)-H(7A)...O(22)#4	0.99	2.48	3.186(3)	128.0
C(7)-H(7B)...O(10)#1	0.99	2.52	3.394(3)	147.5
C(8)-H(8A)...O(22)#4	0.99	2.55	3.268(3)	128.9
C(13)-H(13A)...O(15)#3	0.98	2.64	3.611(4)	171.8
C(19)-H(19A)...O(14)#2	0.98	2.50	3.427(4)	157.5
C(25)-H(25)...O(10)#1	0.95	2.40	3.189(4)	140.8
N(31)-H(31)...O(17)#5	0.88	2.32	3.163(3)	159.1
C(3)-H(3)...O(10)#1	1.00	2.24	3.208(3)	161.3
C(7)-H(7A)...O(22)#4	0.99	2.48	3.186(3)	128.0
C(7)-H(7B)...O(10)#1	0.99	2.52	3.394(3)	147.5
C(8)-H(8A)...O(22)#4	0.99	2.55	3.268(3)	128.9
C(13)-H(13A)...O(15)#3	0.98	2.64	3.611(4)	171.8
C(19)-H(19A)...O(14)#2	0.98	2.50	3.427(4)	157.5
C(25)-H(25)...O(10)#1	0.95	2.40	3.189(4)	140.8
N(31)-H(31)...O(17)#5	0.88	2.32	3.163(3)	159.1
C(3)-H(3)...O(10)#1	1.00	2.24	3.208(3)	161.3
C(7)-H(7A)...O(22)#4	0.99	2.48	3.186(3)	128.0
C(7)-H(7B)...O(10)#1	0.99	2.52	3.394(3)	147.5
C(8)-H(8A)...O(22)#4	0.99	2.55	3.268(3)	128.9
C(13)-H(13A)...O(15)#3	0.98	2.64	3.611(4)	171.8
C(19)-H(19A)...O(14)#2	0.98	2.50	3.427(4)	157.5
C(25)-H(25)...O(10)#1	0.95	2.40	3.189(4)	140.8
N(31)-H(31)...O(17)#5	0.88	2.32	3.163(3)	159.1
C(3)-H(3)...O(10)#1	1.00	2.24	3.208(3)	161.3
C(7)-H(7A)...O(22)#4	0.99	2.48	3.186(3)	128.0
C(7)-H(7B)...O(10)#1	0.99	2.52	3.394(3)	147.5
C(8)-H(8A)...O(22)#4	0.99	2.55	3.268(3)	128.9
C(13)-H(13A)...O(15)#3	0.98	2.64	3.611(4)	171.8
C(19)-H(19A)...O(14)#2	0.98	2.50	3.427(4)	157.5
C(25)-H(25)...O(10)#1	0.95	2.40	3.189(4)	140.8
N(31)-H(31)...O(17)#5	0.88	2.32	3.163(3)	159.1
C(3)-H(3)...O(10)#1	1.00	2.24	3.208(3)	161.3
C(7)-H(7A)...O(22)#4	0.99	2.48	3.186(3)	128.0
C(7)-H(7B)...O(10)#1	0.99	2.52	3.394(3)	147.5

C(8)-H(8A)...O(22)#4	0.99	2.55	3.268(3)	128.9
C(13)-H(13A)...O(15)#3	0.98	2.64	3.611(4)	171.8
C(19)-H(19A)...O(14)#2	0.98	2.50	3.427(4)	157.5
C(25)-H(25)...O(10)#1	0.95	2.40	3.189(4)	140.8
N(31)-H(31)...O(17)#5	0.88	2.32	3.163(3)	159.1
C(3)-H(3)...O(10)#1	1.00	2.24	3.208(3)	161.3
C(7)-H(7A)...O(22)#4	0.99	2.48	3.186(3)	128.0
C(7)-H(7B)...O(10)#1	0.99	2.52	3.394(3)	147.5
C(8)-H(8A)...O(22)#4	0.99	2.55	3.268(3)	128.9
C(13)-H(13A)...O(15)#3	0.98	2.64	3.611(4)	171.8
C(19)-H(19A)...O(14)#2	0.98	2.50	3.427(4)	157.5
C(25)-H(25)...O(10)#1	0.95	2.40	3.189(4)	140.8

Symmetry transformations used to generate equivalent atoms:

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

#4 x+1,y,z #5 x,y+1,z