Supporting Information Appendix

Asymmetric Total Synthesis of (+)-(2*R*,4'*R*,8'*R*)-α-Tocopherol Enabled by Enzymatic Desymmetrization

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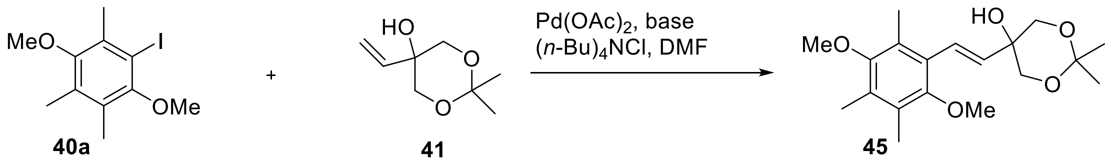
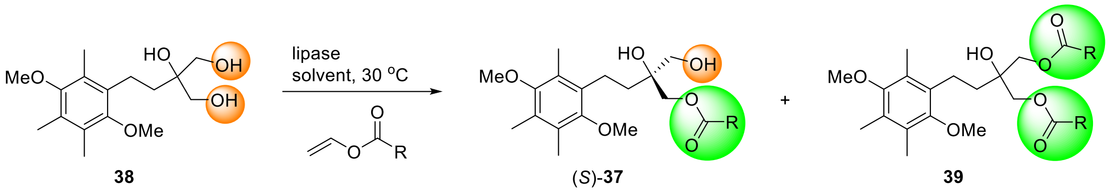
Table S1. Screening conditions for the Heck coupling between 40a and 41[a]



Entry	Base	Conversion (%)[b]	Yield of **45** (%)[b]
1	NEt_3	23.3	23.3
2	$NaHCO_3$	74.3	74.3
3	Na_2CO_3	98.5	98.5 (85.0[c])
4	Ag_2CO_3	8.6	8.6
5	Cs_2CO_3	89.0	74.2

[a]Reaction conditions: **40a** (0.16 mmol), **41** (0.20 mmol, 1.25 equiv.), $Pd(OAc)_2$ (0.008 mmol, 0.05 equiv.), base (0.65 mmol, 4 equiv.), $(n\text{-}Bu)_4NCl$ (0.21 mmol, 1.3 equiv.) in DMF (1.0 mL). [b]Determined by GC-MS analysis. [c]Isolated yield.

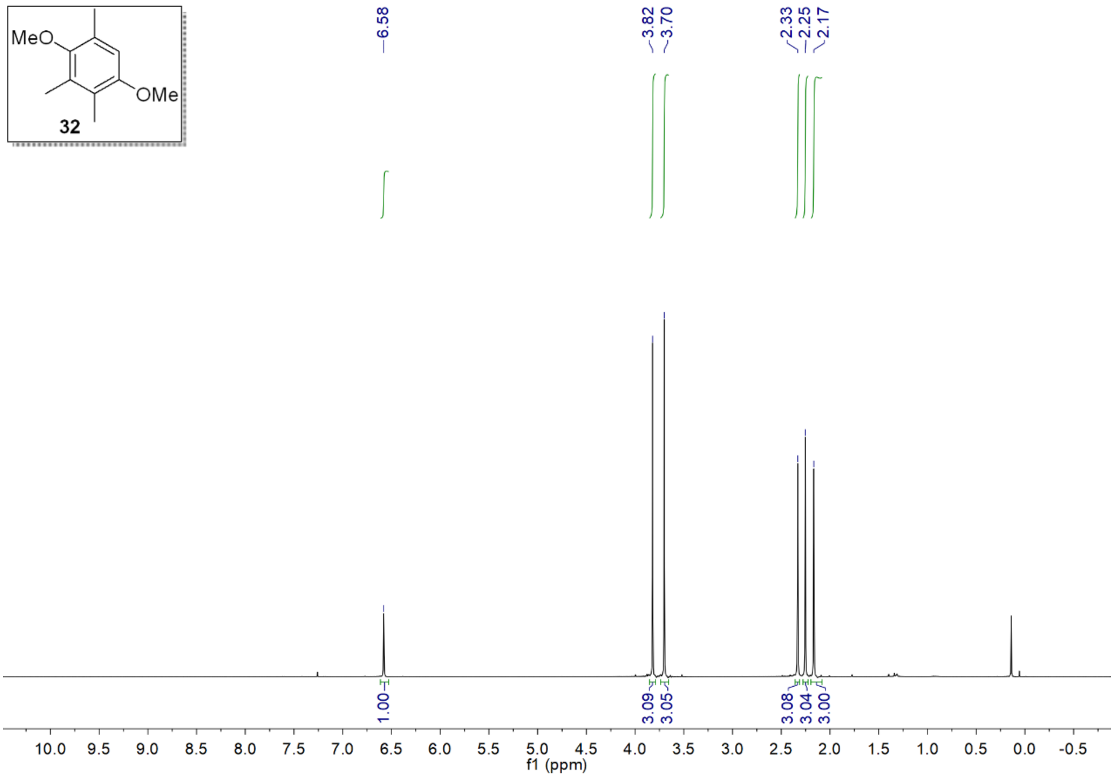
Table S2. Enzymatic desymmetric transesterification of triol 38[a]



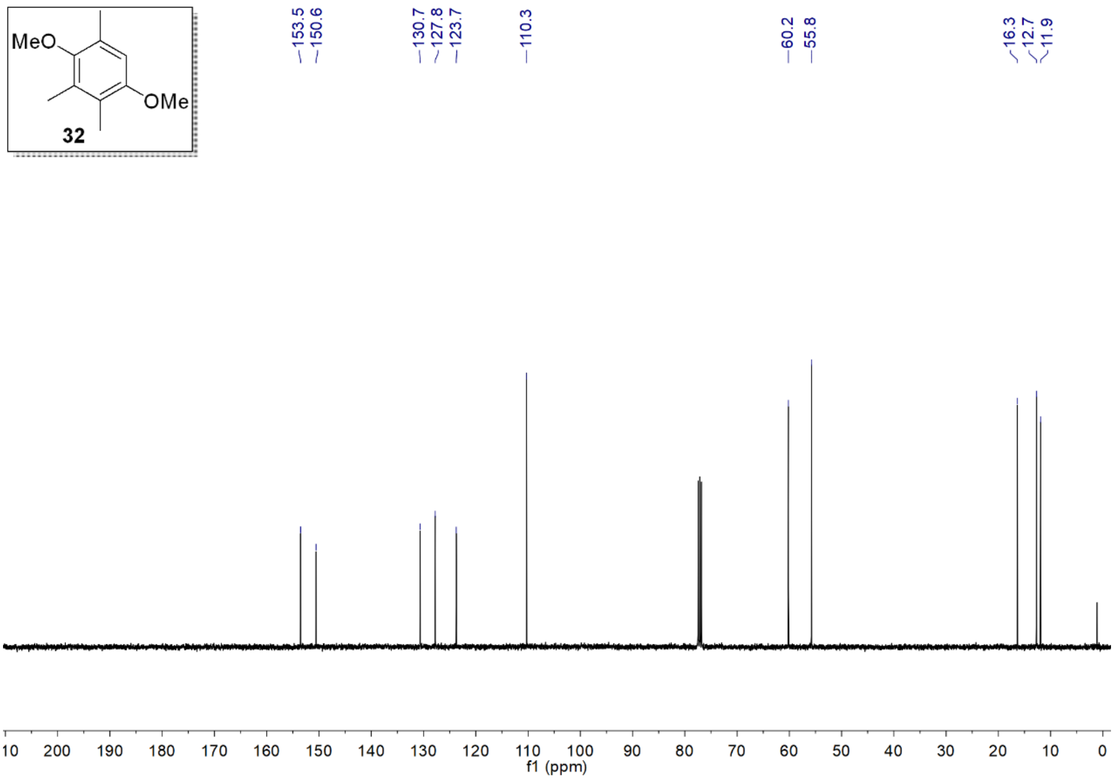
Entry	Lipase	R	Solvent	**38** remaining (%)[b]	Yield of (*S*)-**37** (%)[b]	Yield of **39** (%)[b]	Ee of (*S*)-**37** (%)[b]
1	PPL	Me	Et_2O	60.1	39.9	0	85.7
2	lipase-M	Me	Et_2O	87.8	12.2	0	63.5
3	PPL	Ph	Et_2O	81.7	18.3	0	56.9
4	lipase-M	Ph	Et_2O	95.6	4.4	0	ND[c]
5	PPL	Pr	Et_2O	10.3	88.3	1.2	89.9
6	lipase-M	Pr	Et_2O	70.4	29.6	0	62.6
7	lipase-PF	Pr	Et_2O	47.8	45.1	7.1	34.5
8	lipase-PS	Pr	Et_2O	95.8	4.2	0	ND
9	lipase-G	Pr	Et_2O	96.7	3.3	0	ND
10	lipase-N	Pr	Et_2O	0	4.5	95.5	11.9
11	PPL	Pr	$(i\text{-Pr})_2O$	0.3	90.1	9.6	>99

[a]Reaction conditions (1 mL): **38** (3 mg), lipase (3 mg), and transesterification reagent (0.1 mmol) in solvent. Reaction mixtures were incubated at 30 °C with 200 rpm shaking for 12 h. [b]Determined by chiral HPLC analysis. [c]Not determined.

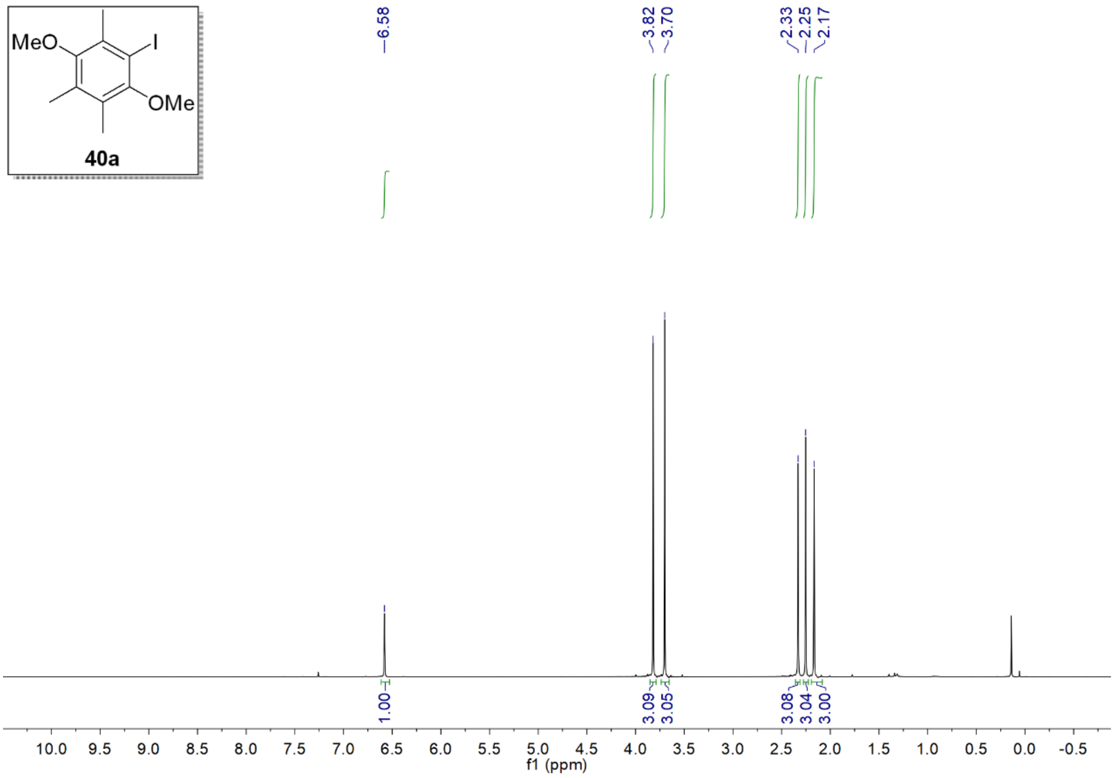
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of 32



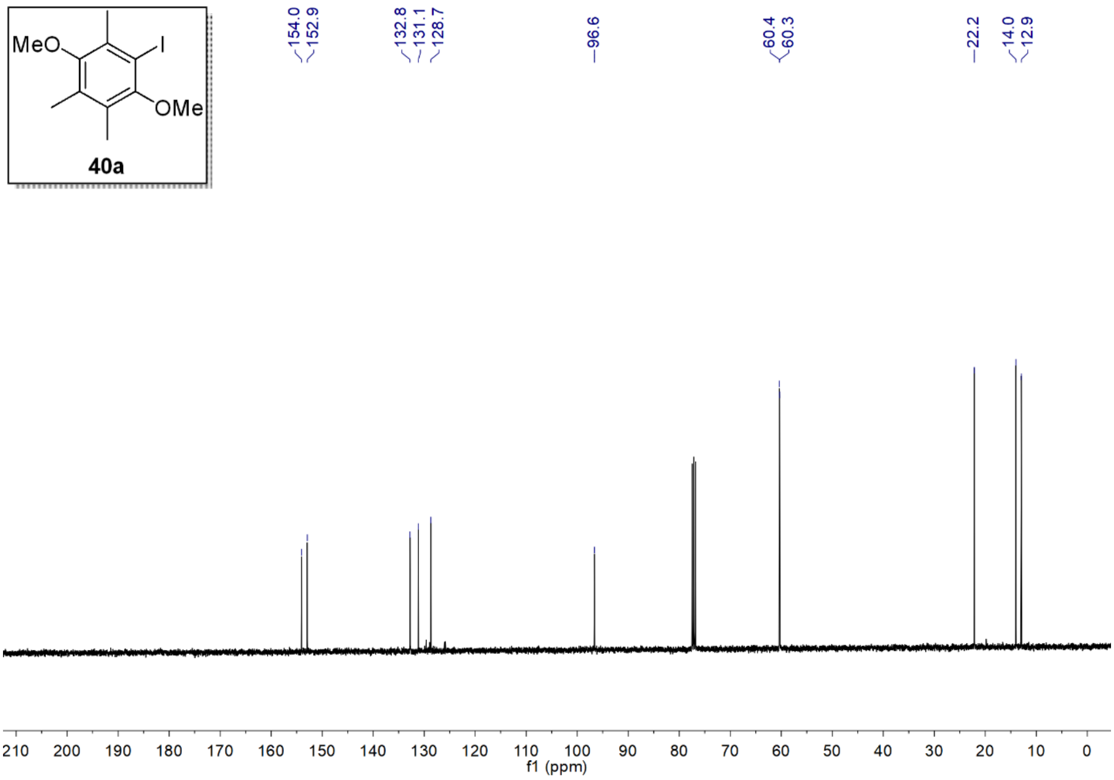
The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of 32



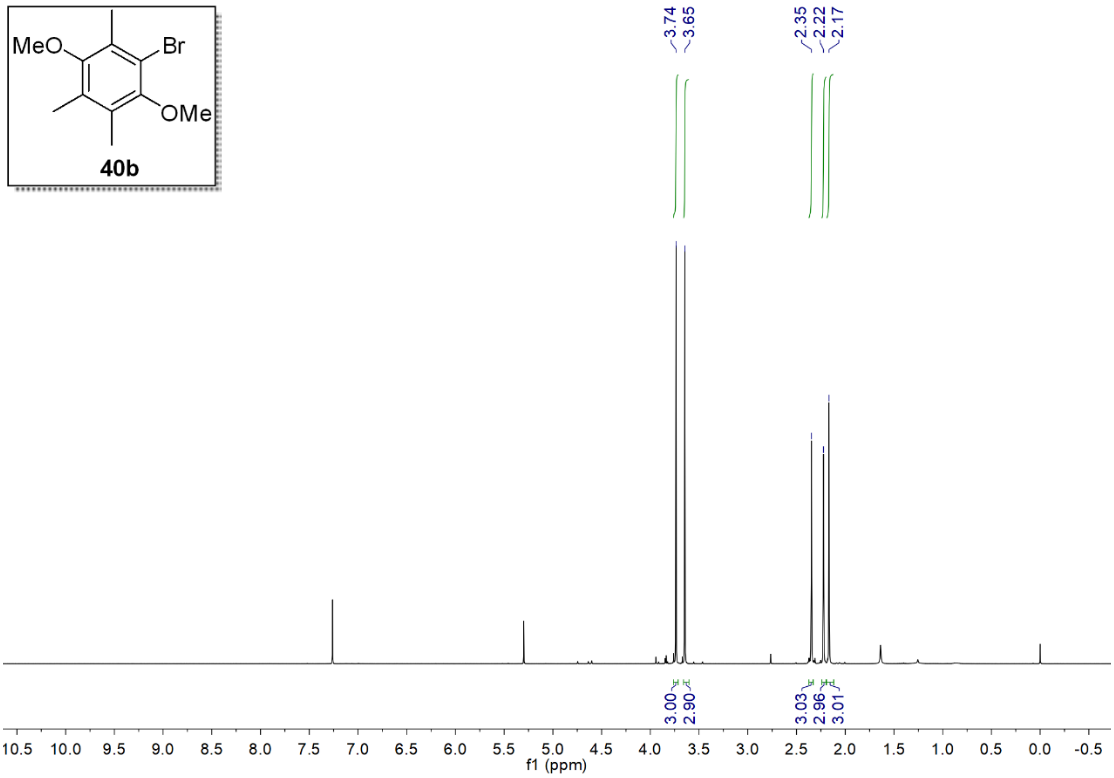
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of 40a



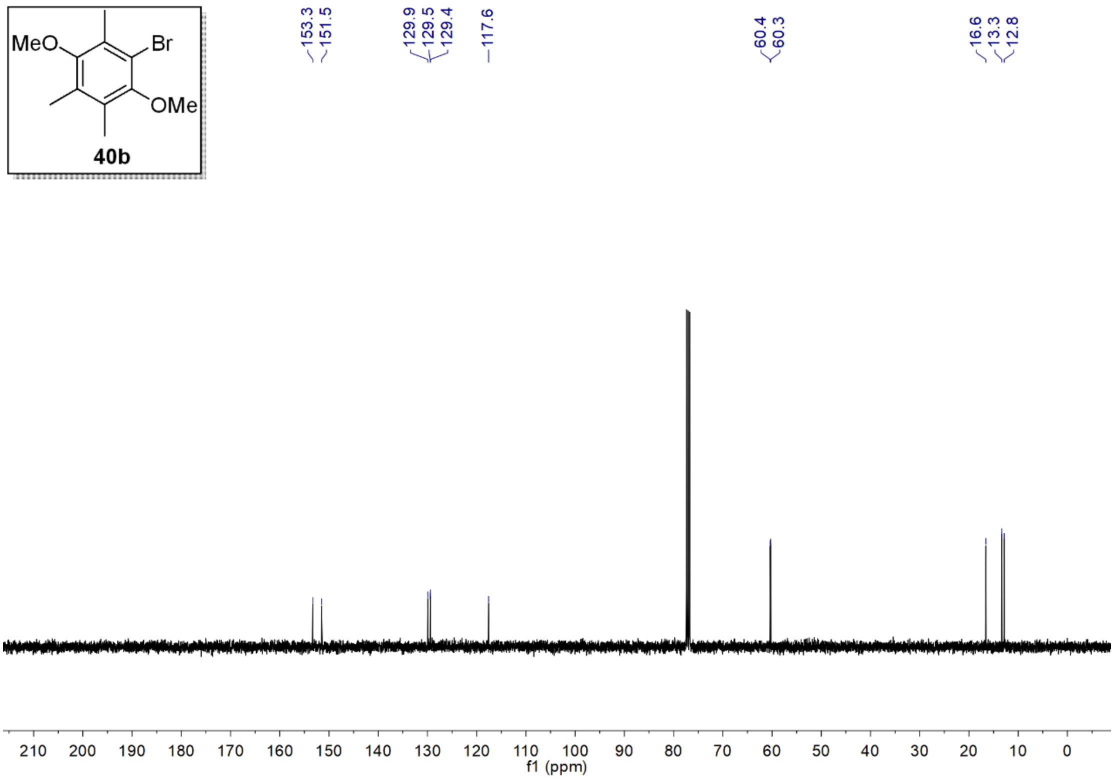
The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of 40a



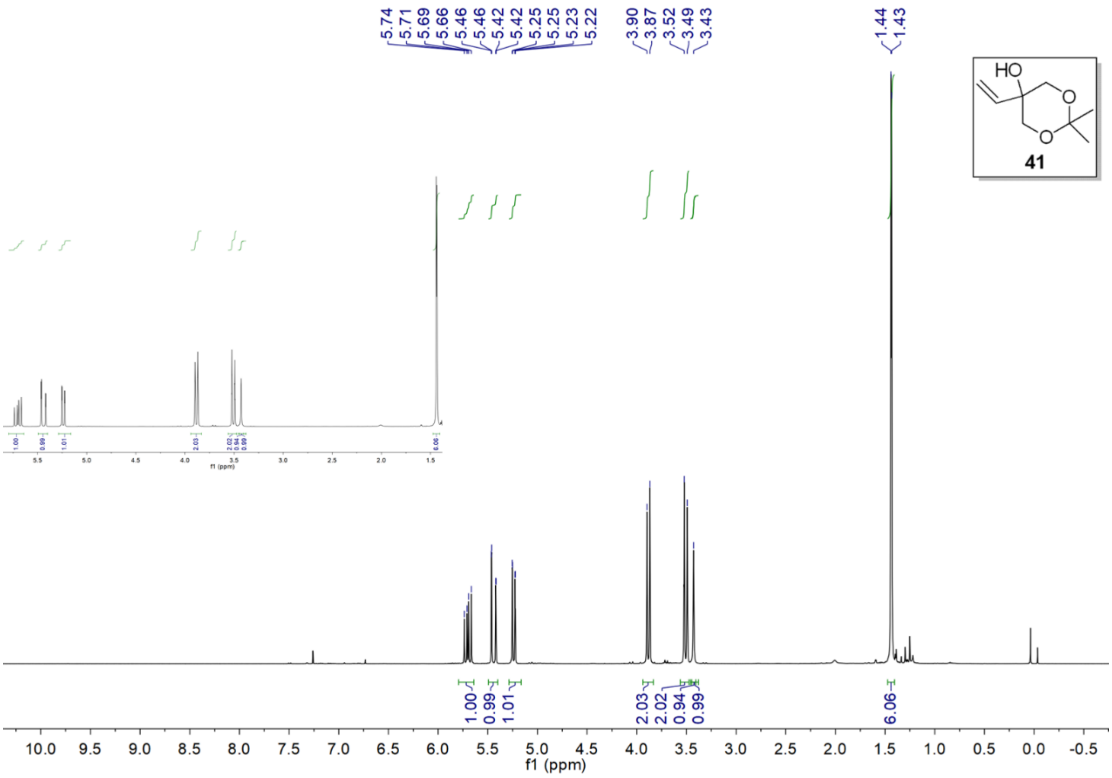
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of 40b



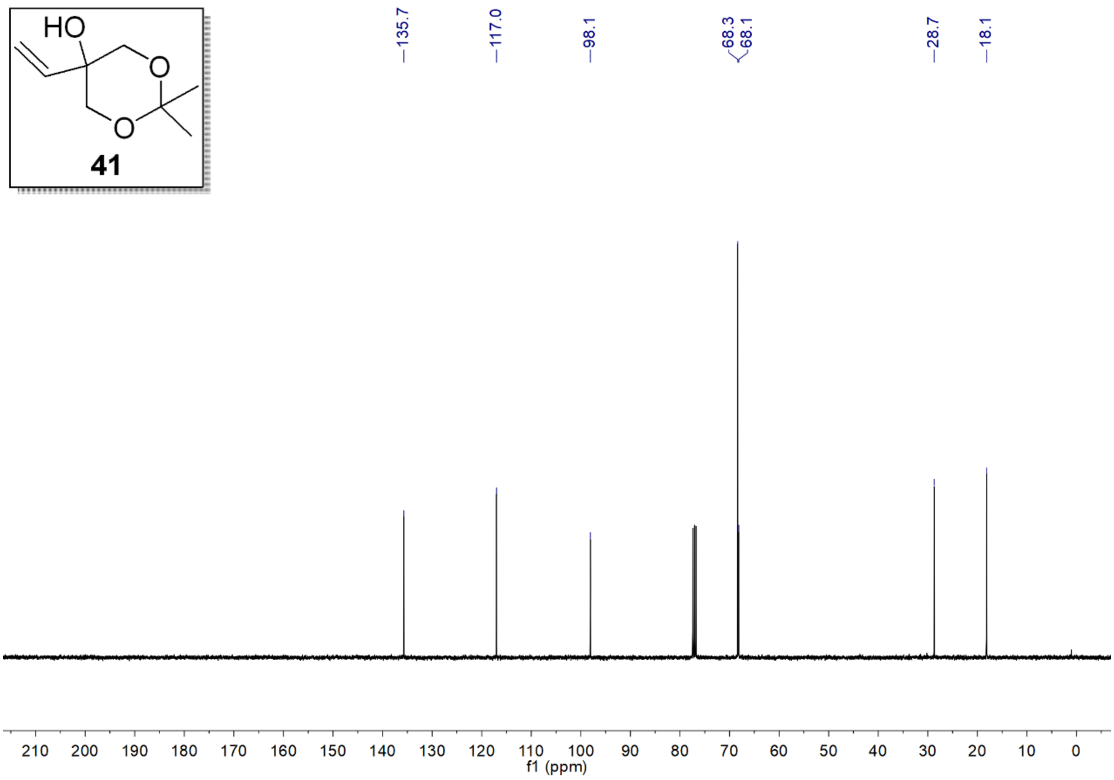
The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of 40b



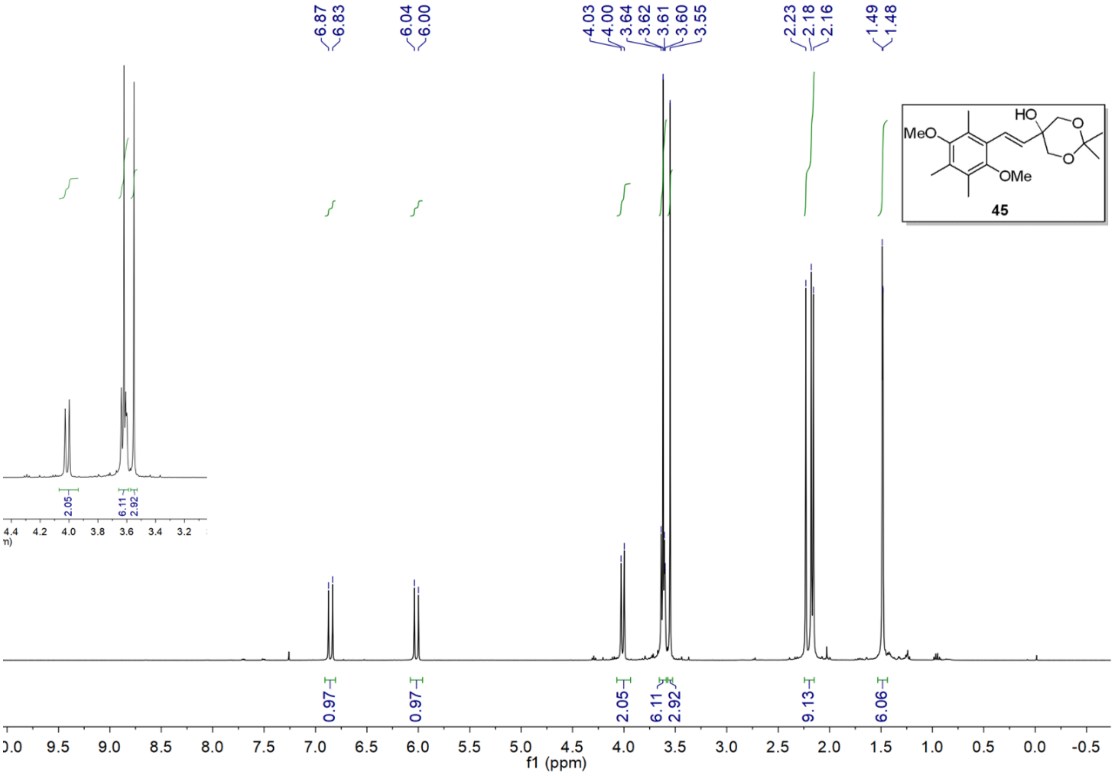
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of 41



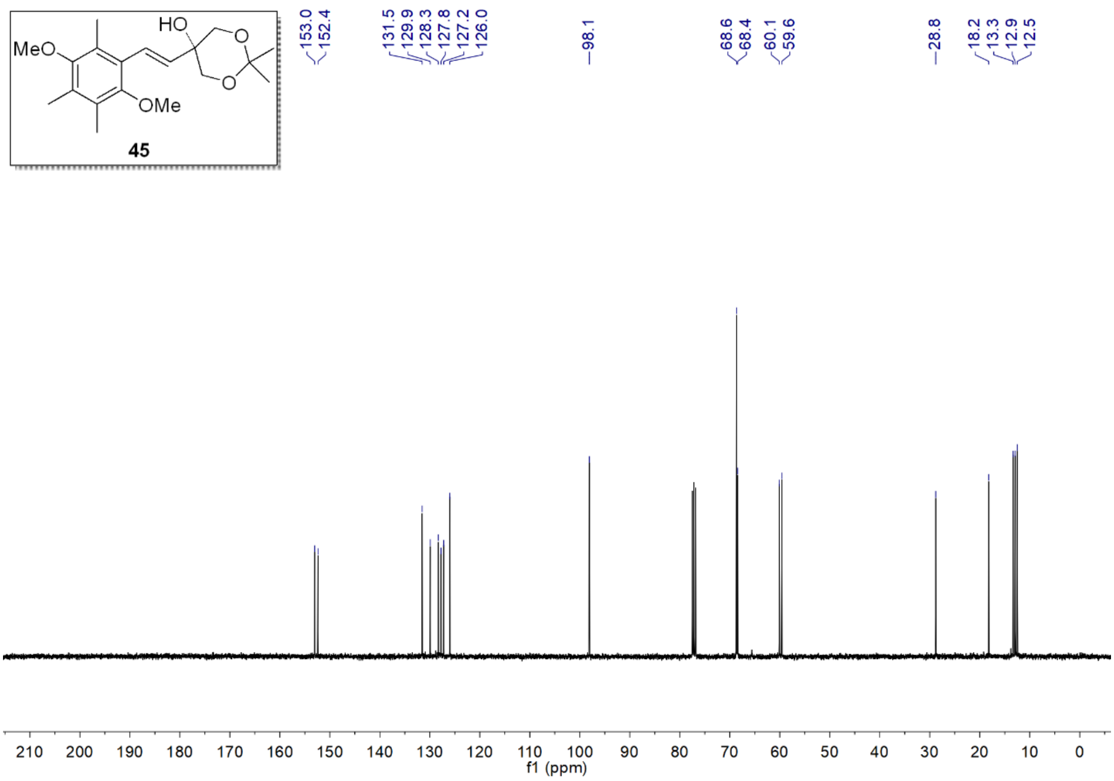
The ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) Spectrum of 41



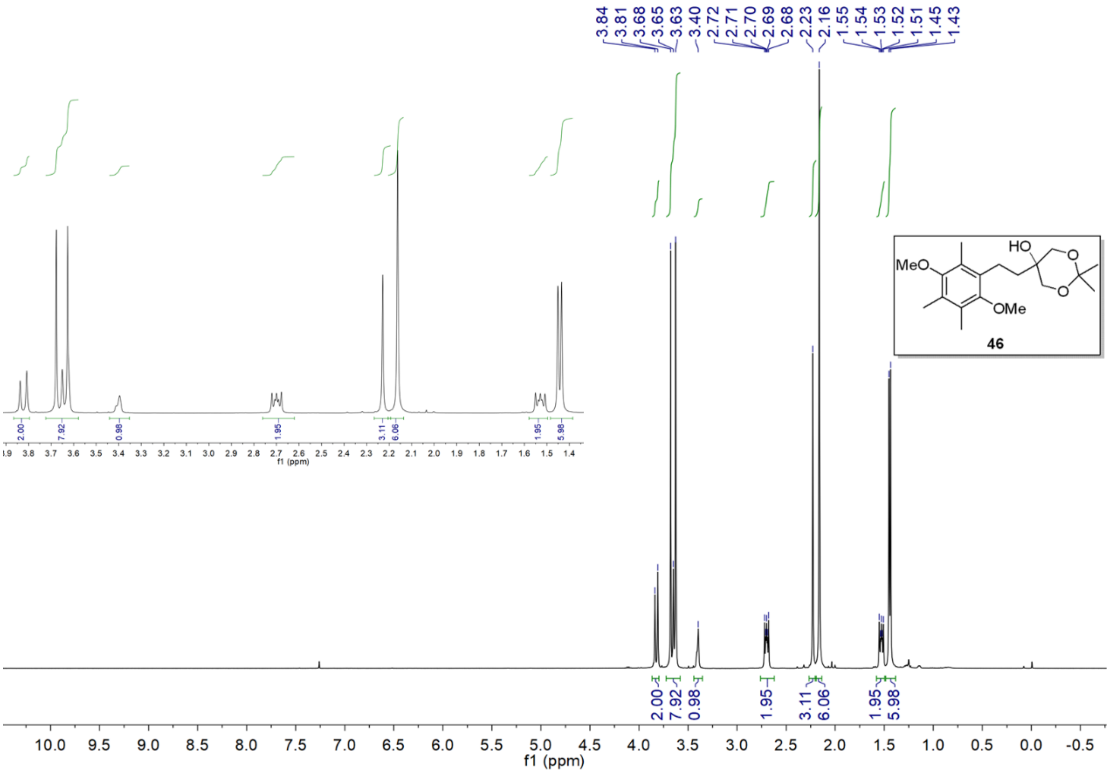
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of 45



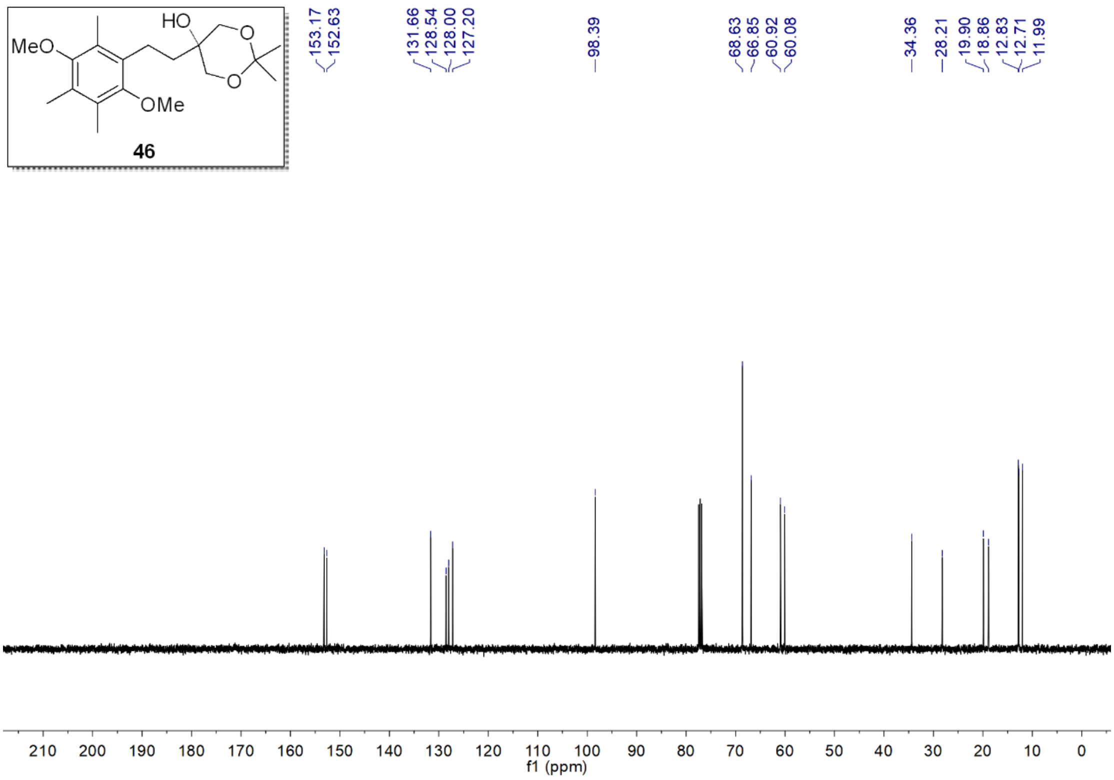
The ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) Spectrum of 45



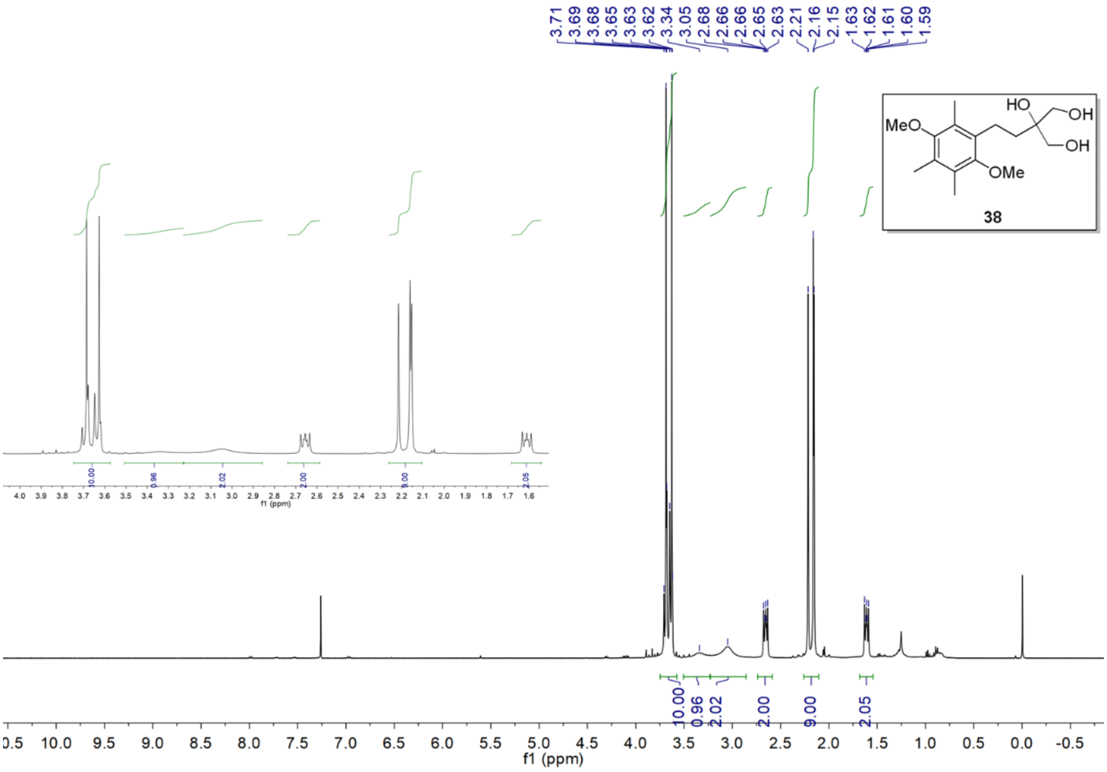
The ¹H NMR (400 MHz, CDCl₃) Spectrum of 46



The ¹³C{¹H} NMR (100 MHz, CDCl₃) Spectrum of 46



The [1]H NMR (400 MHz, CDCl₃) Spectrum of 38



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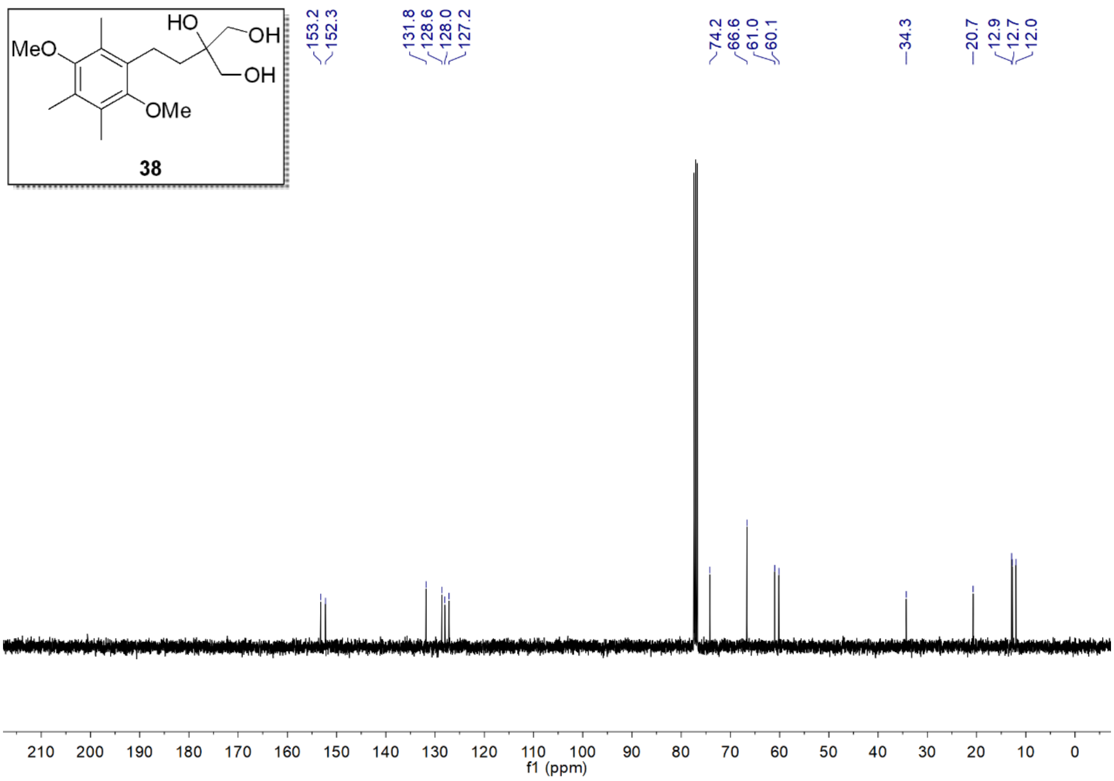
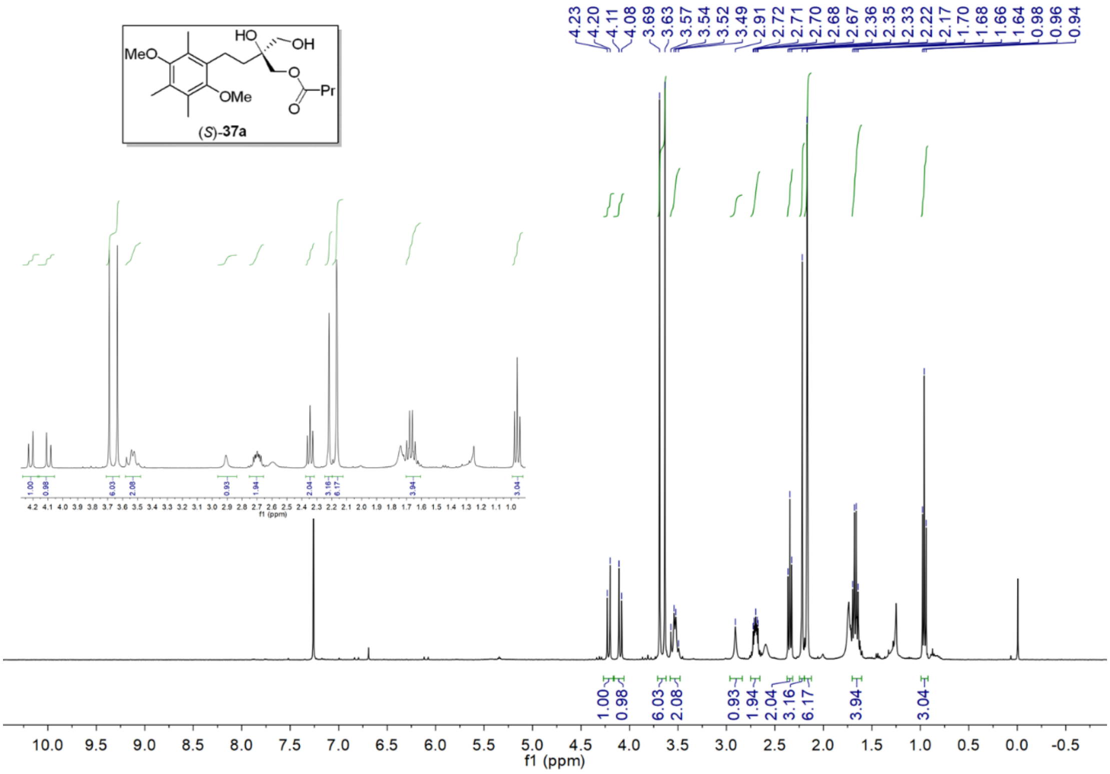
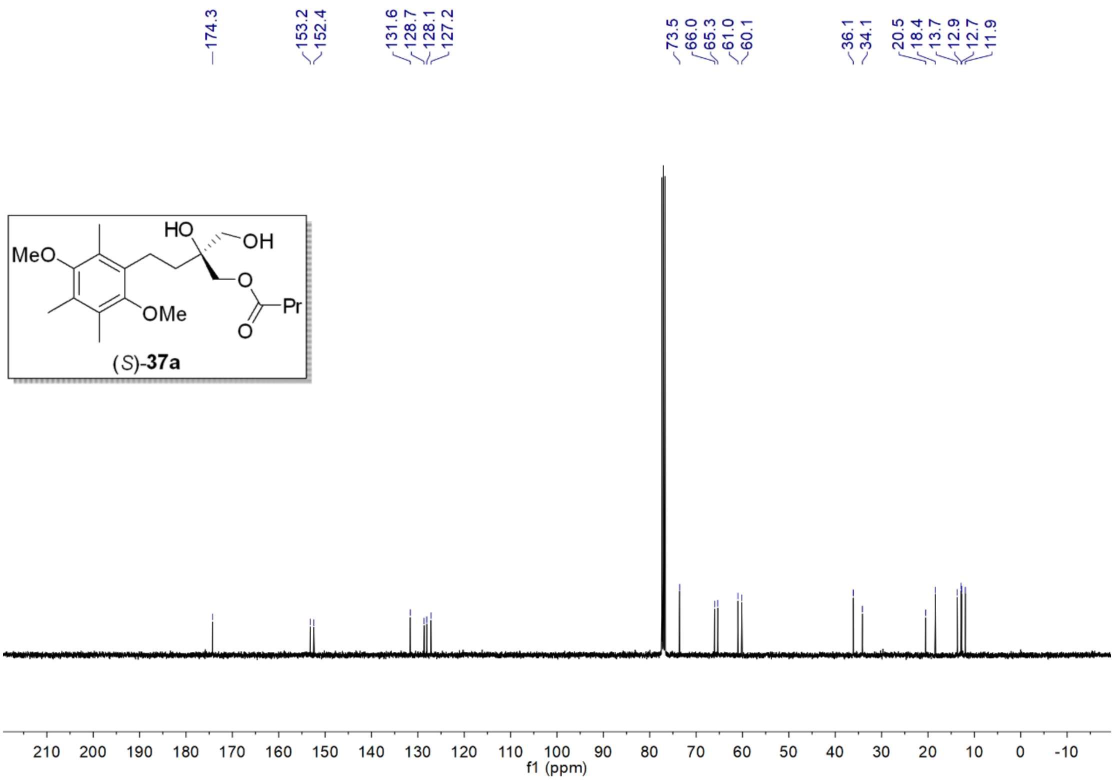
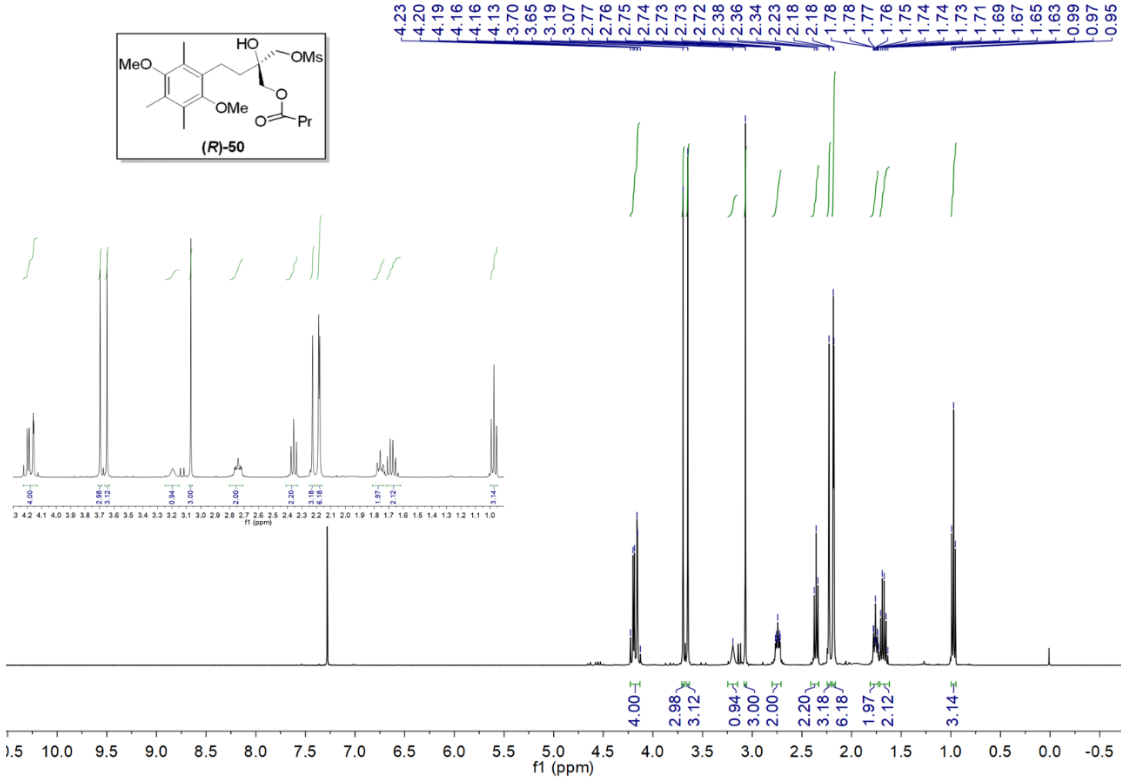


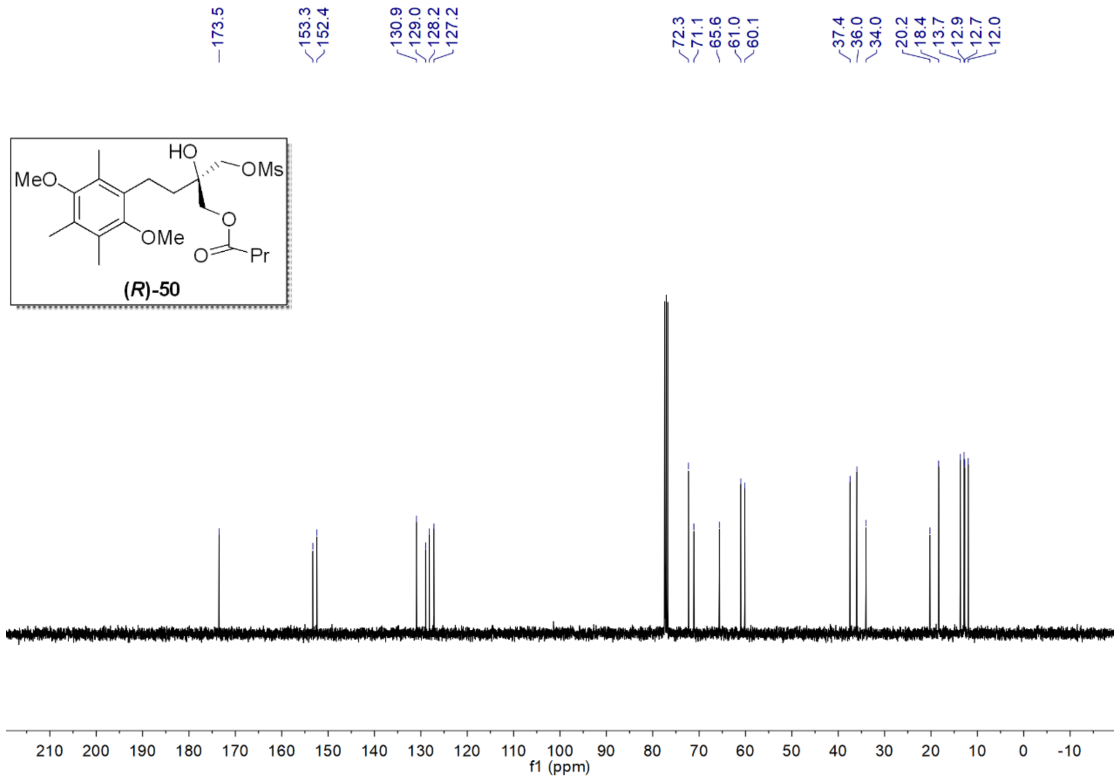
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of (*S*)-37a



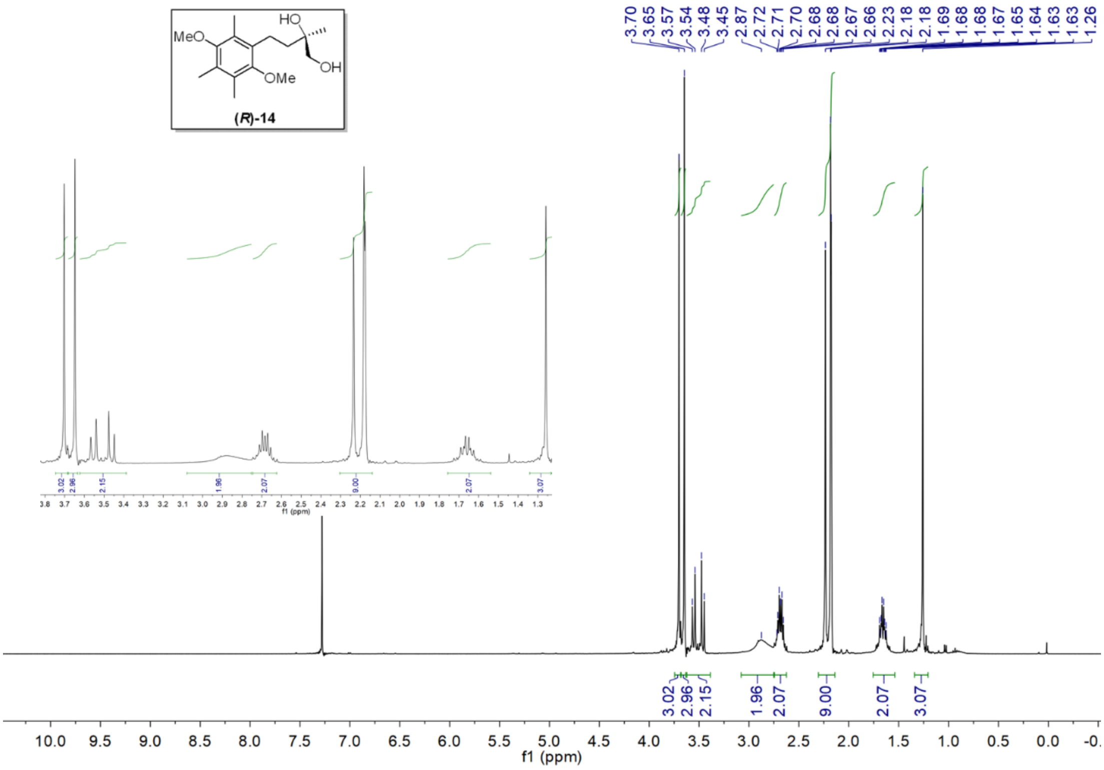
The ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) Spectrum of (*S*)-37a



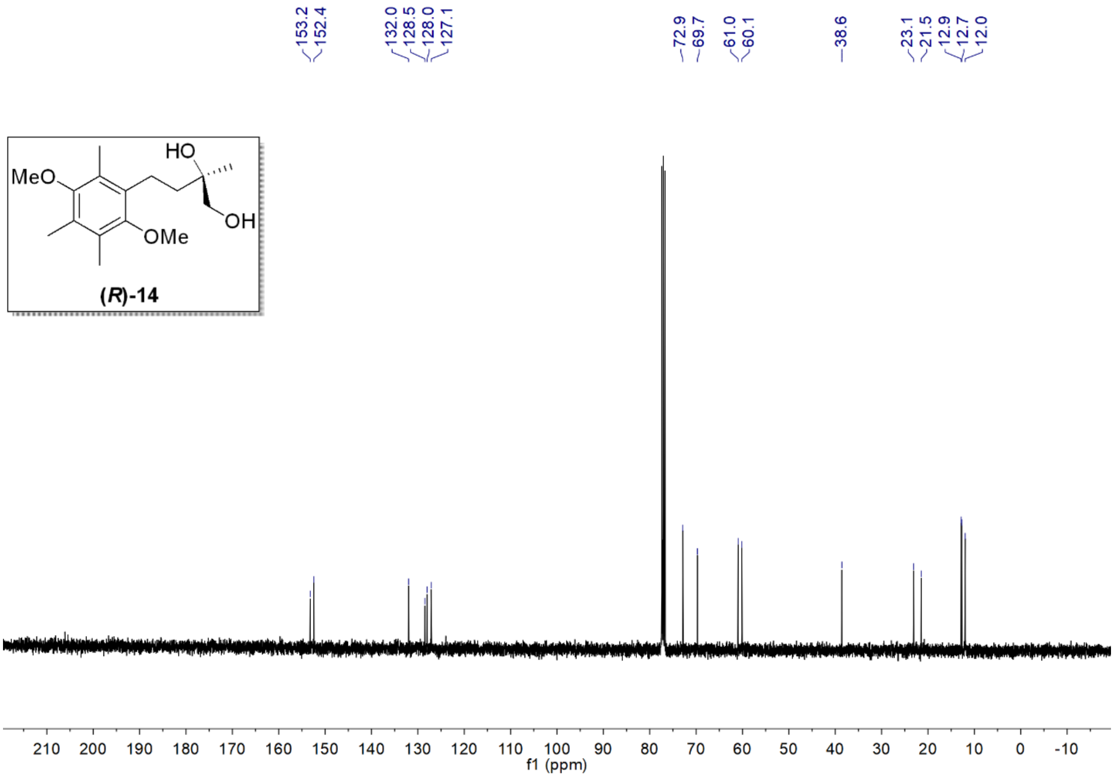


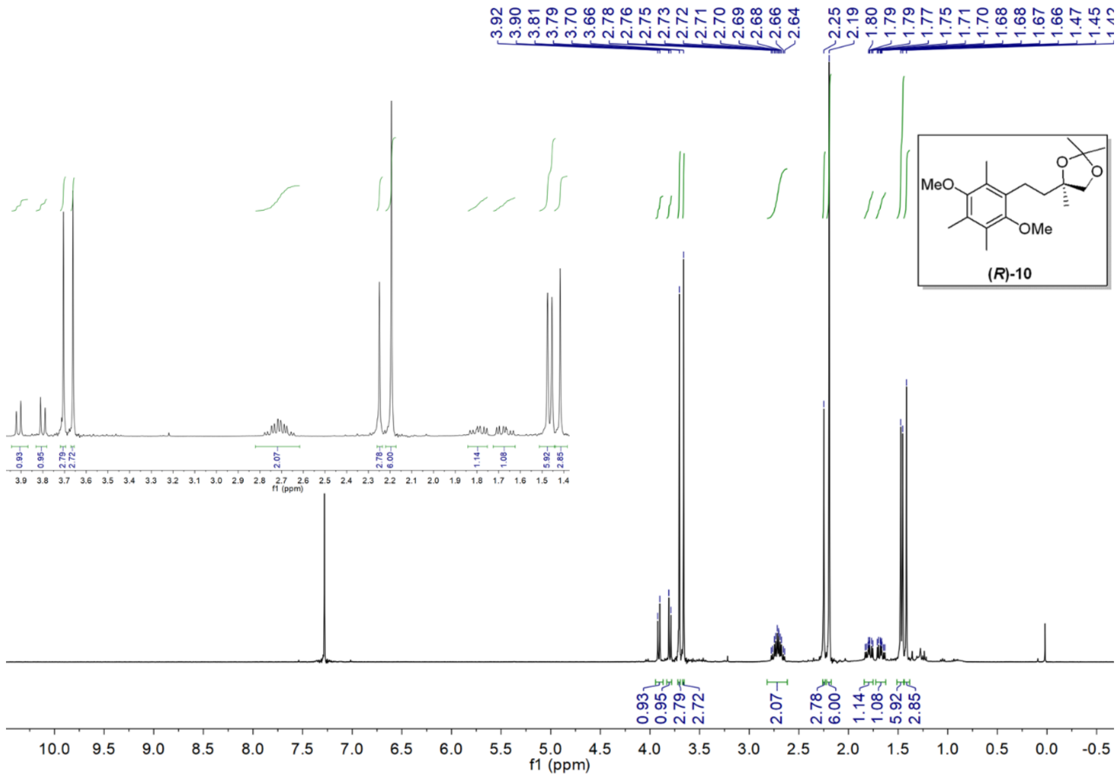


The ^{1}H NMR (400 MHz, CDCl$_3$) Spectrum of (*R*)-14



The ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) Spectrum of (*R*)-14

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MeO
OMe
O
O
(R)-10
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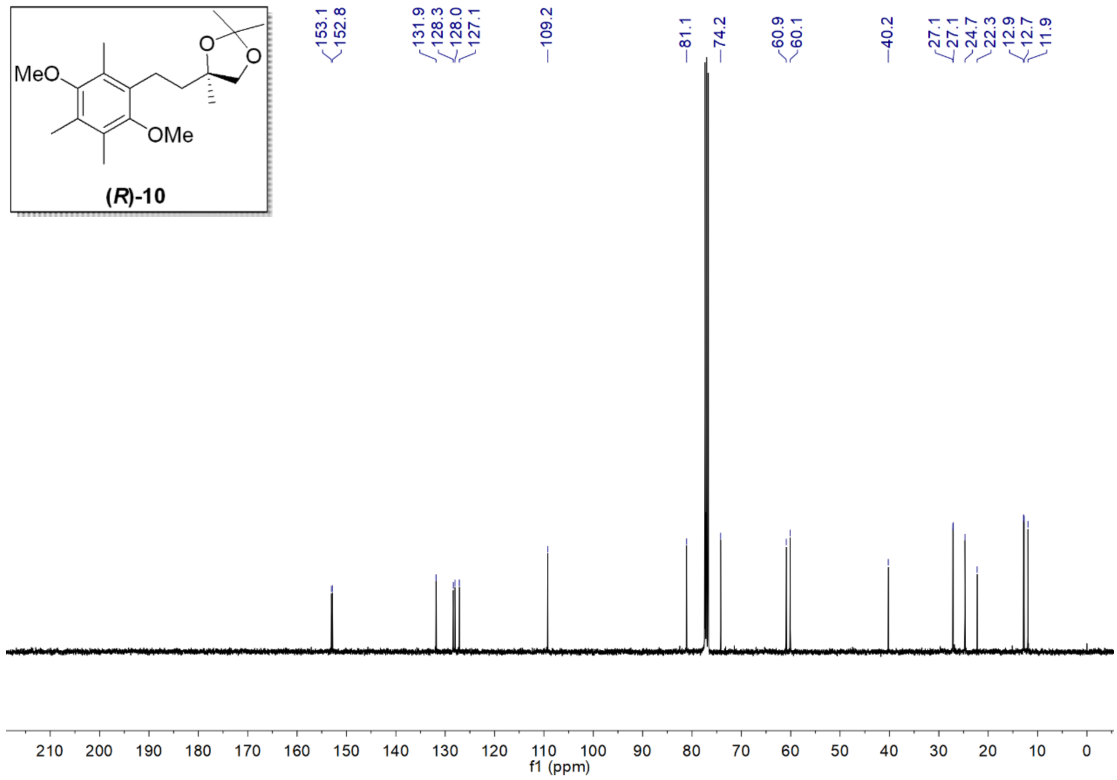
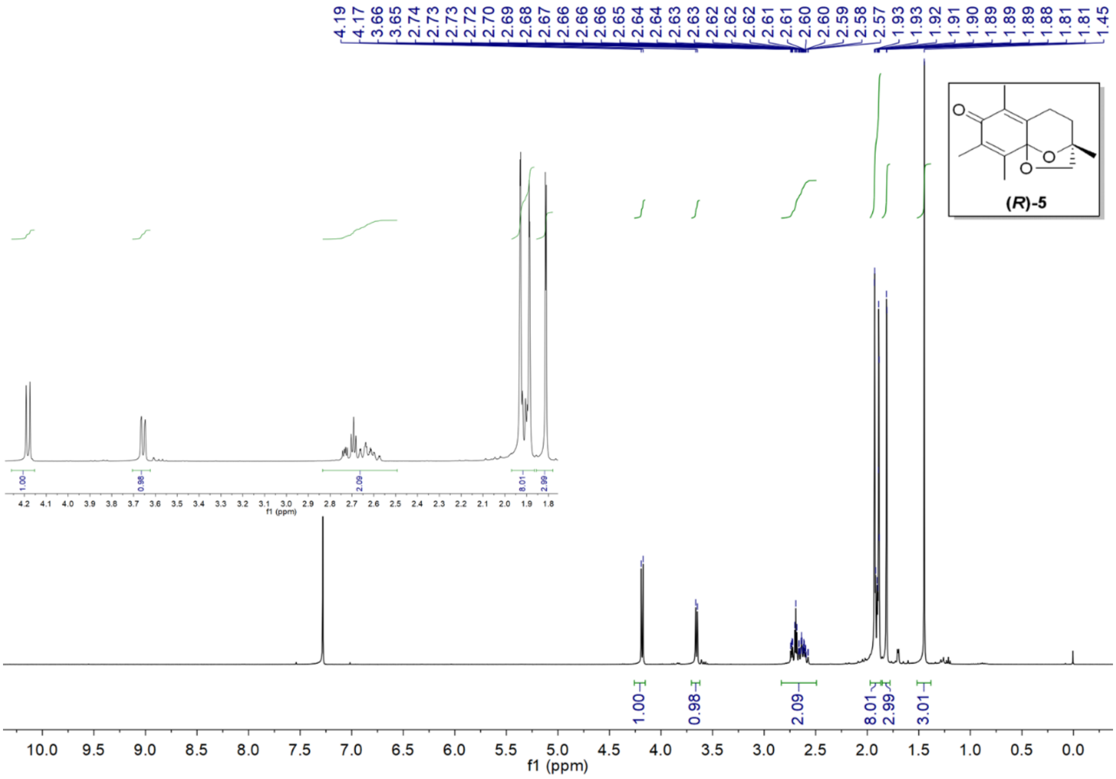
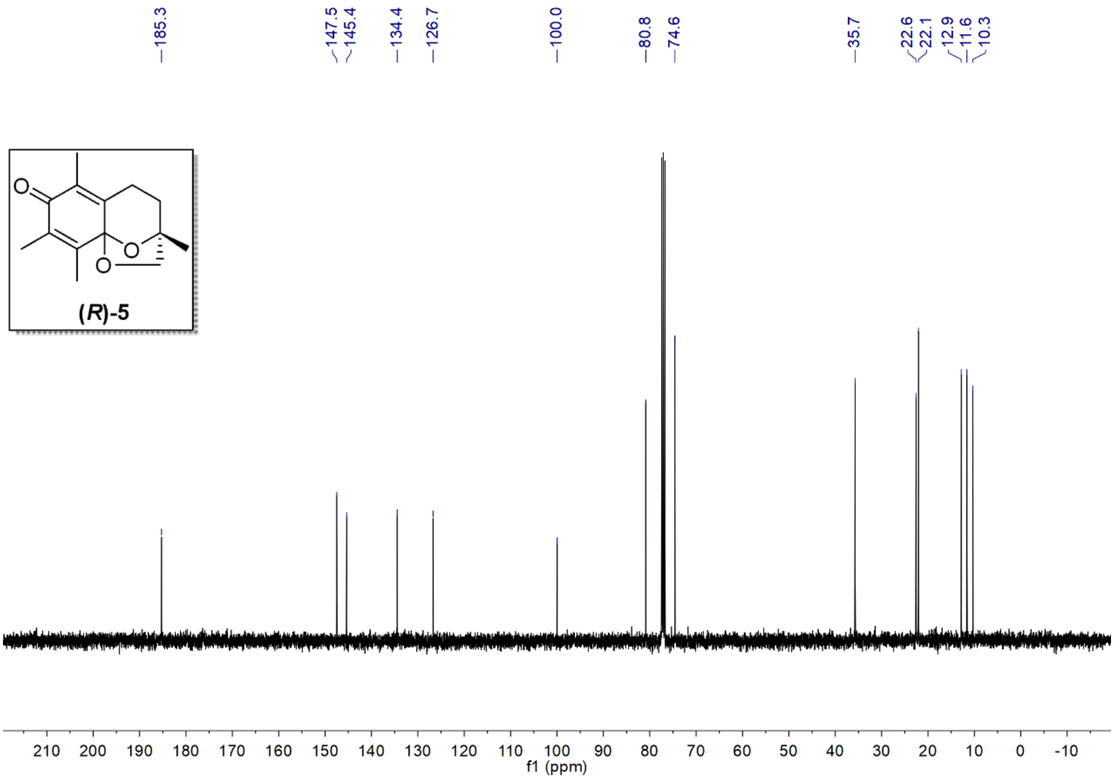
f1 (ppm)


MeO
OMe
O
O
(R)-10
153.1 152.8 131.9 128.3 128.0 127.1 109.2 81.1 74.2 60.9 60.1 40.2 27.1 27.1 24.7 22.3 12.9 12.7 11.9
f1 (ppm)

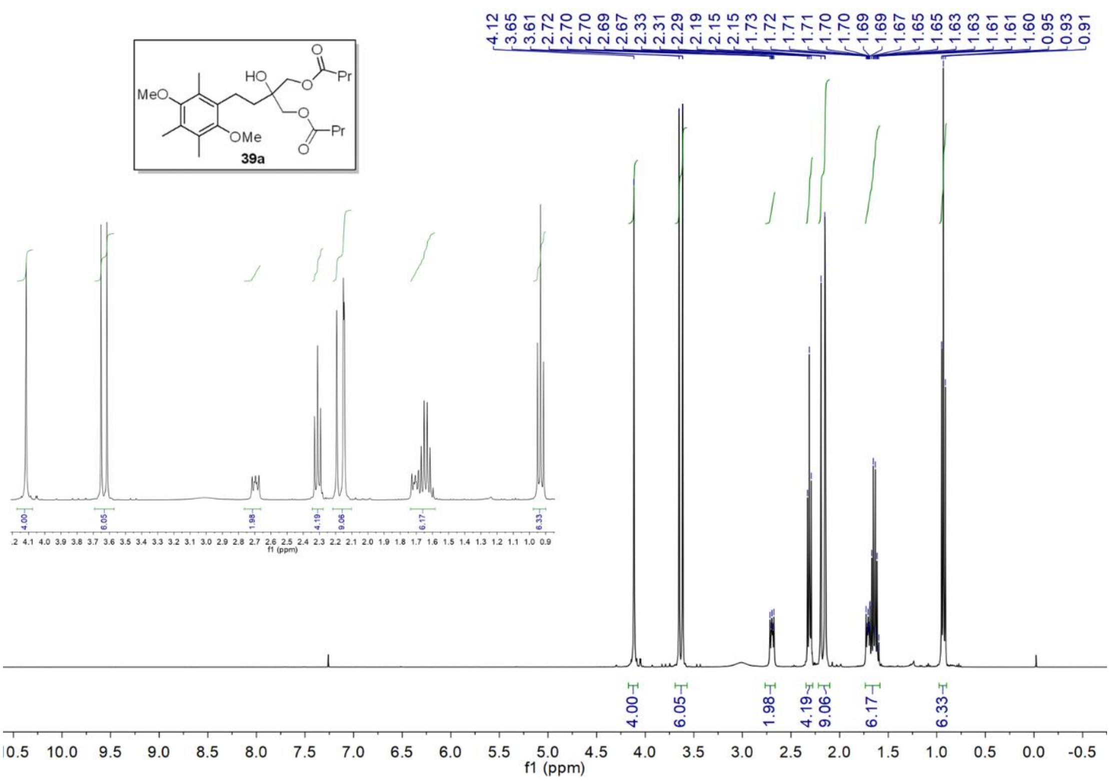
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of (*R*)-5



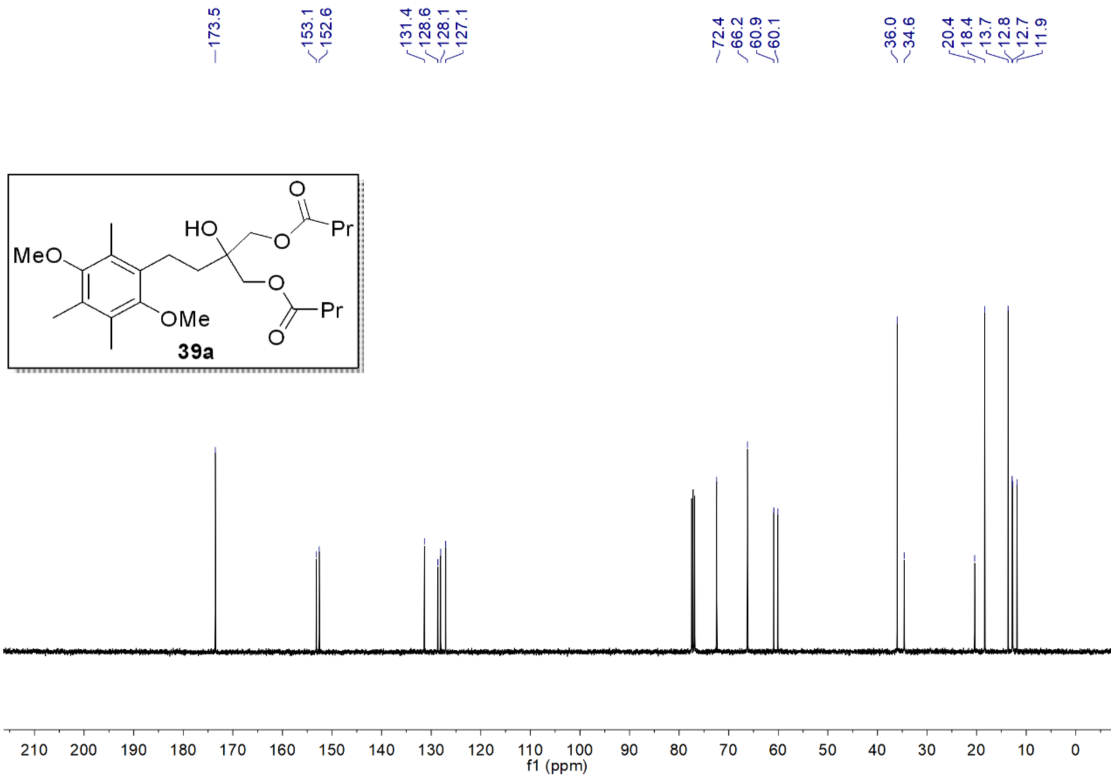
The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of (*R*)-5



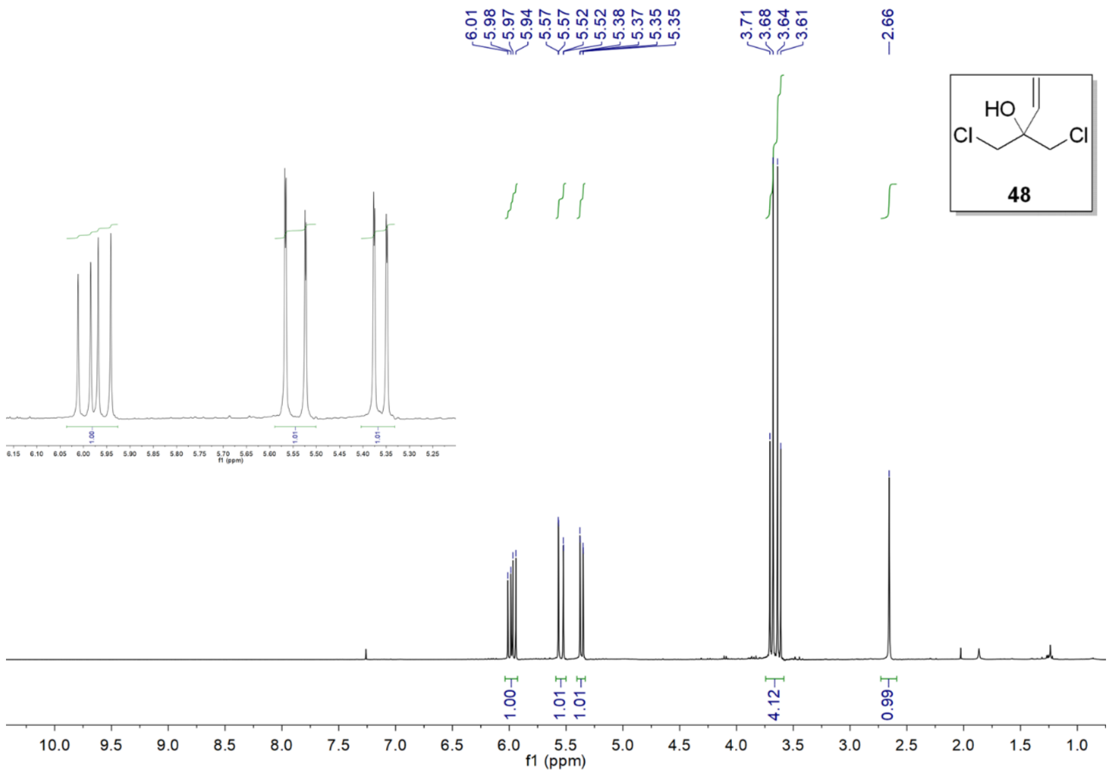
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of 39a



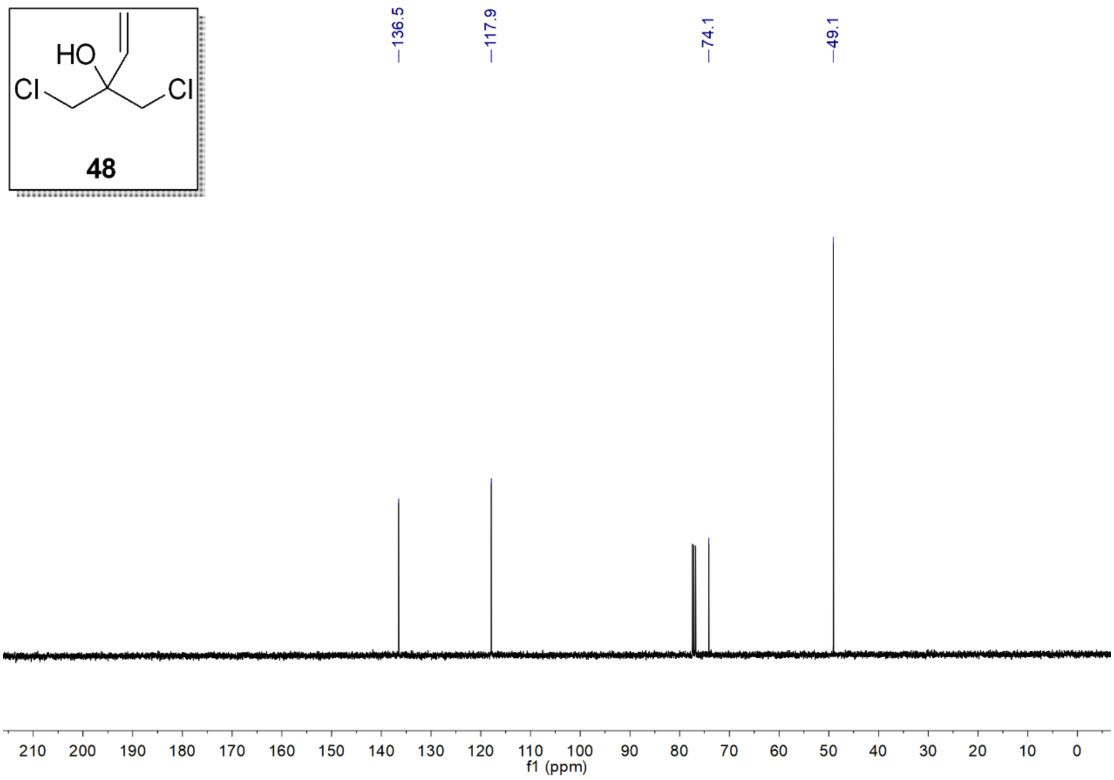
The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of 39a



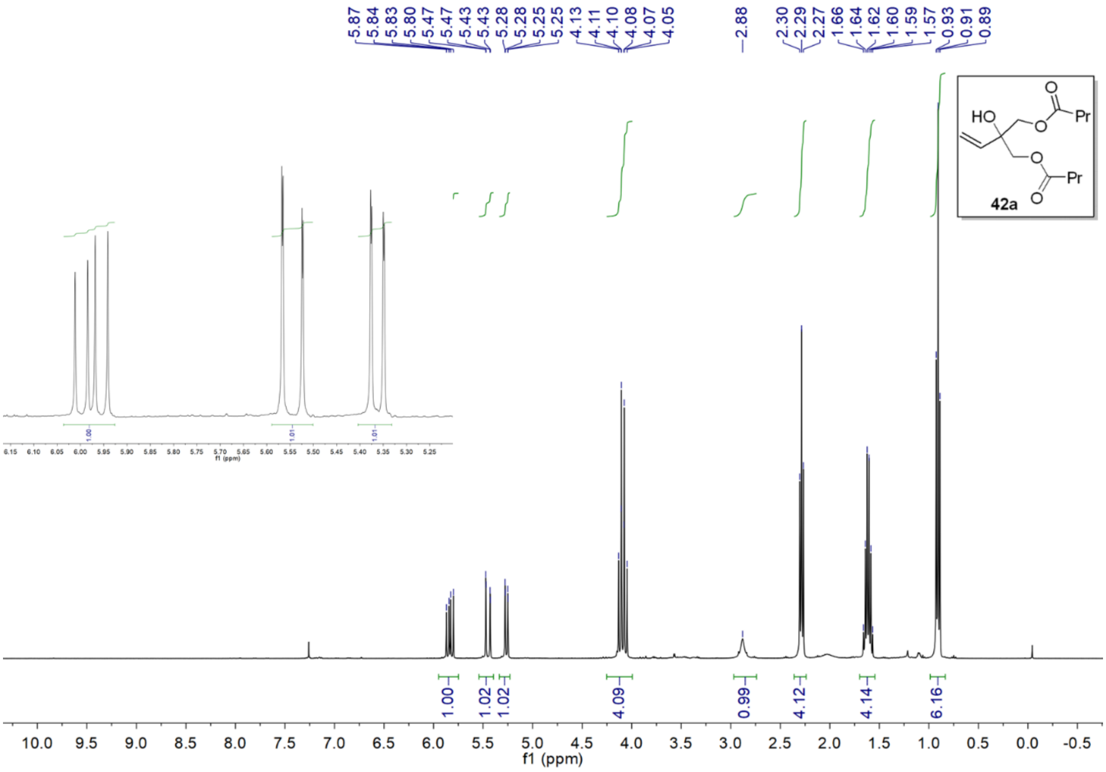
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of 48



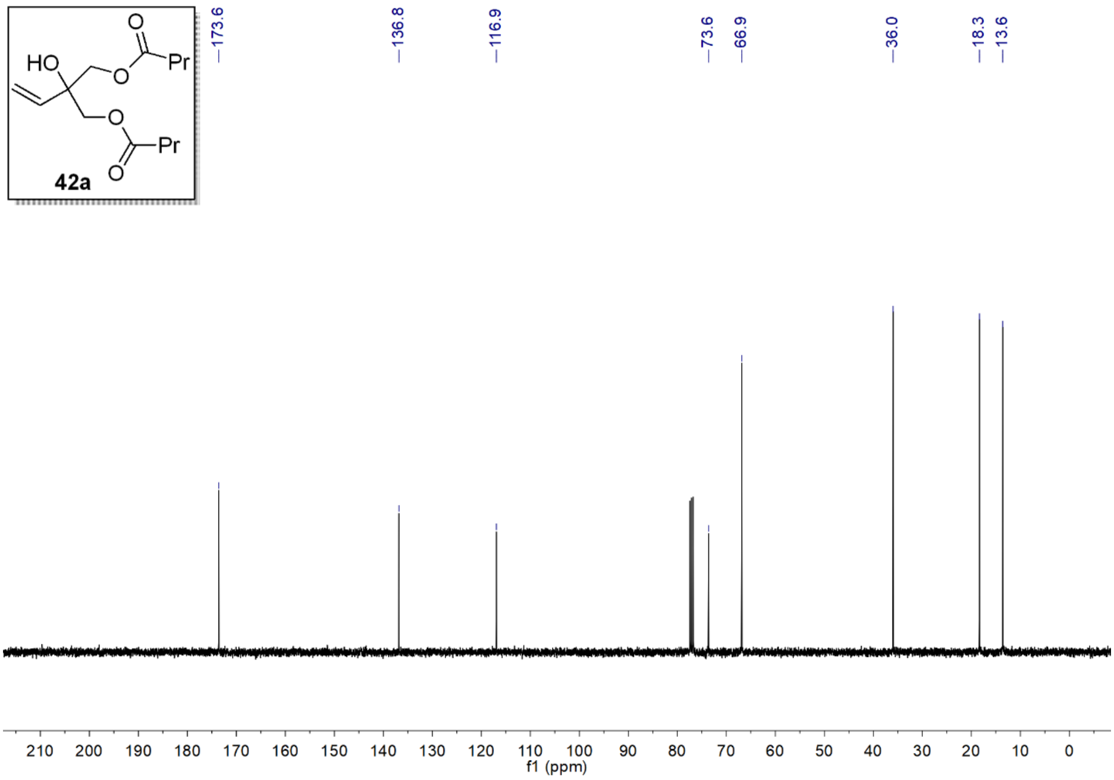
The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of 48



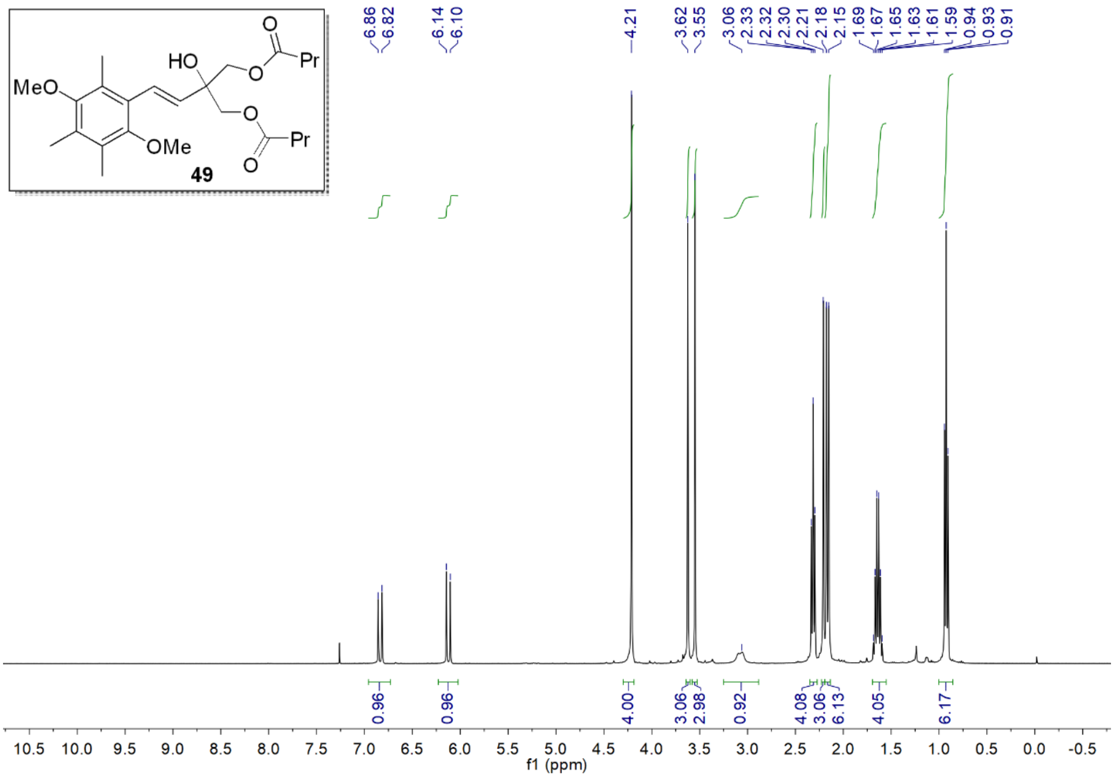
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of 42a



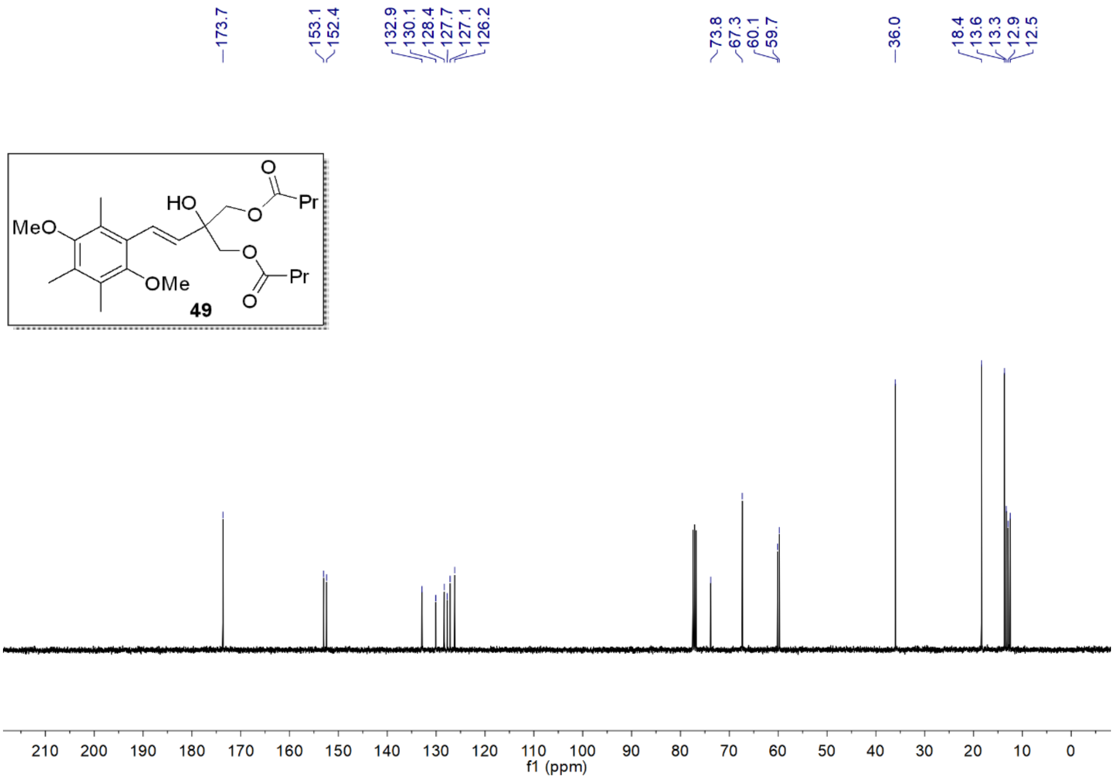
The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of 42a



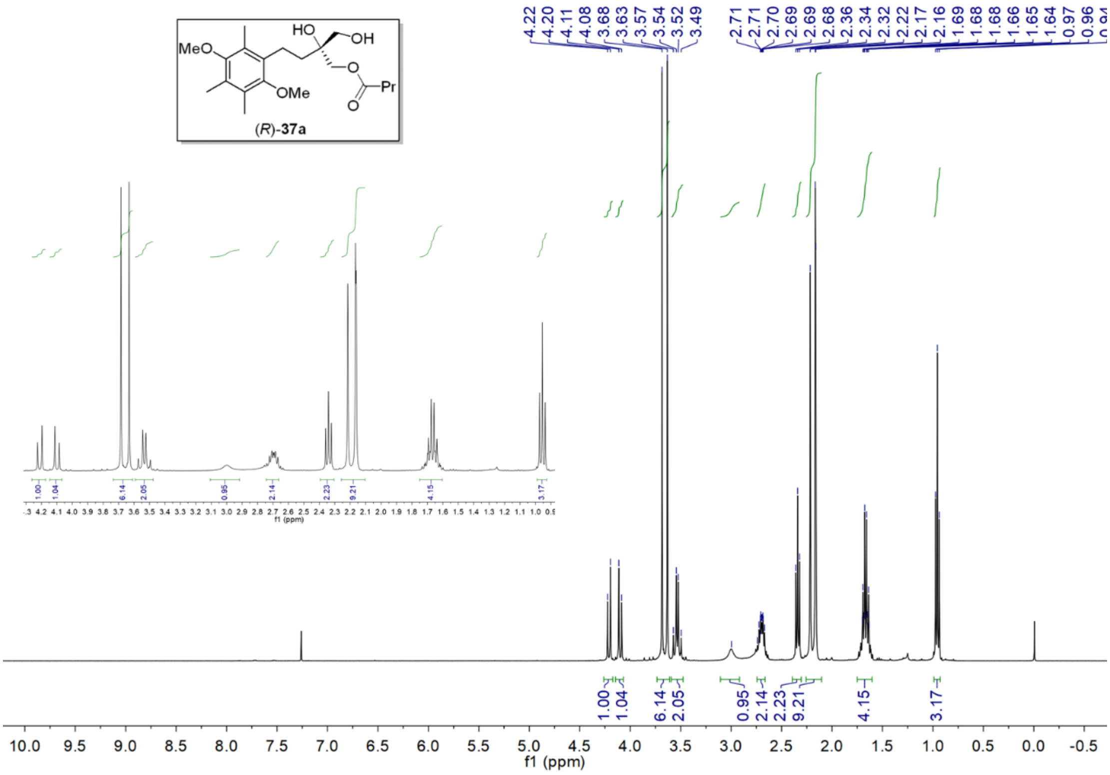
The ¹H NMR (400 MHz, $CDCl_3$) Spectrum of 49



The ¹³C{¹H} NMR (100 MHz, $CDCl_3$) Spectrum of 49



The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of (*R*)-37a



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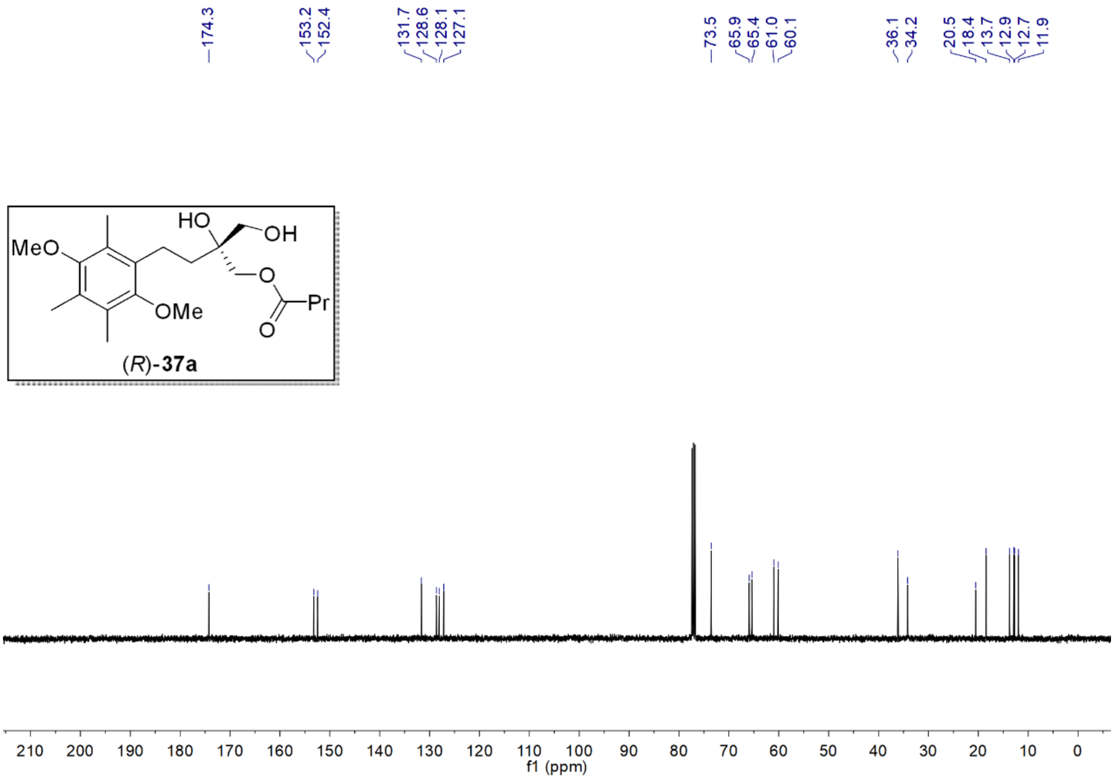
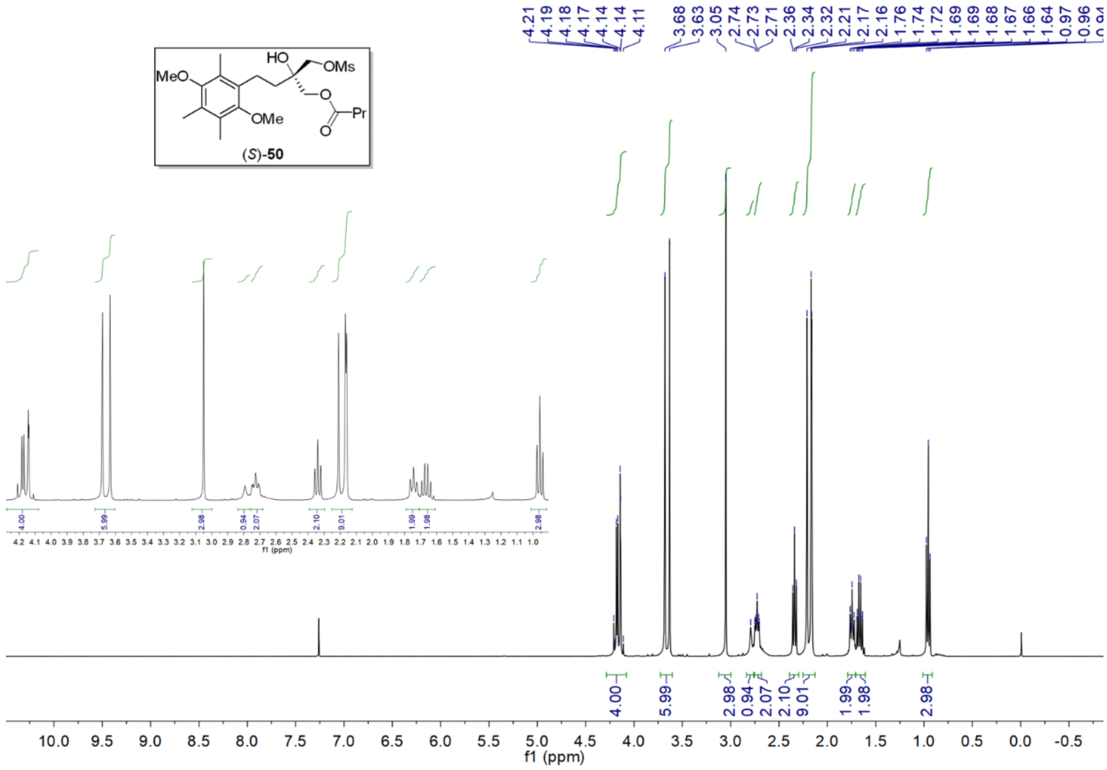
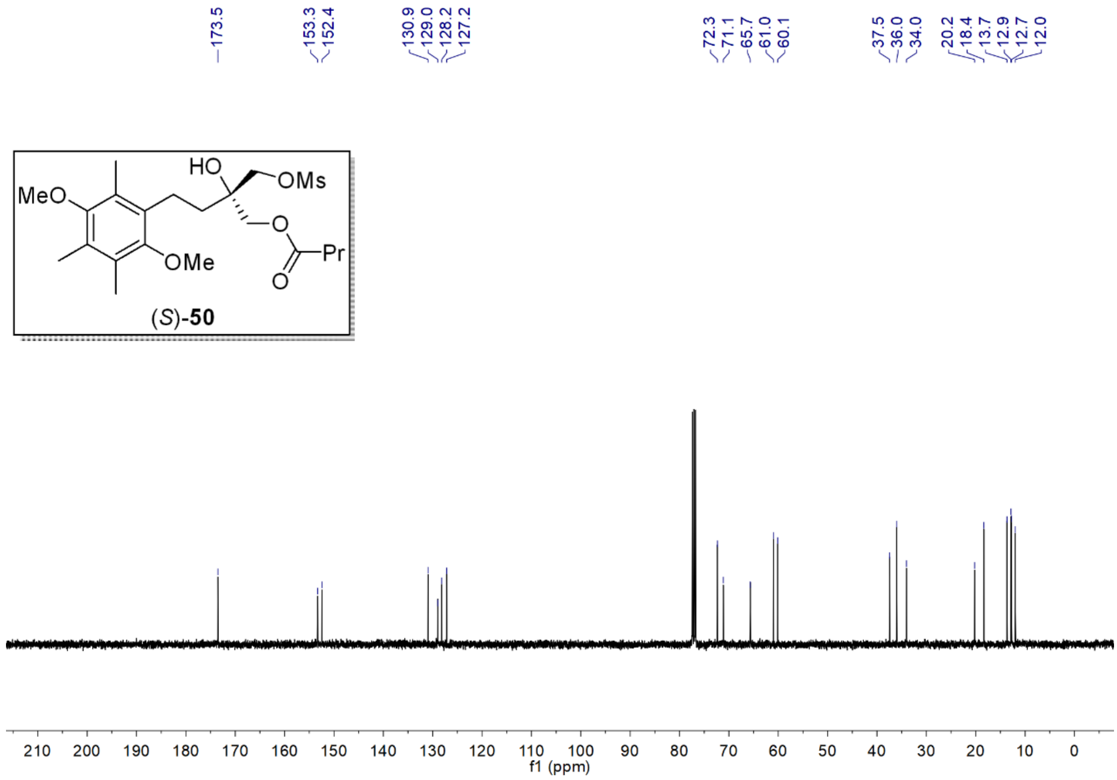


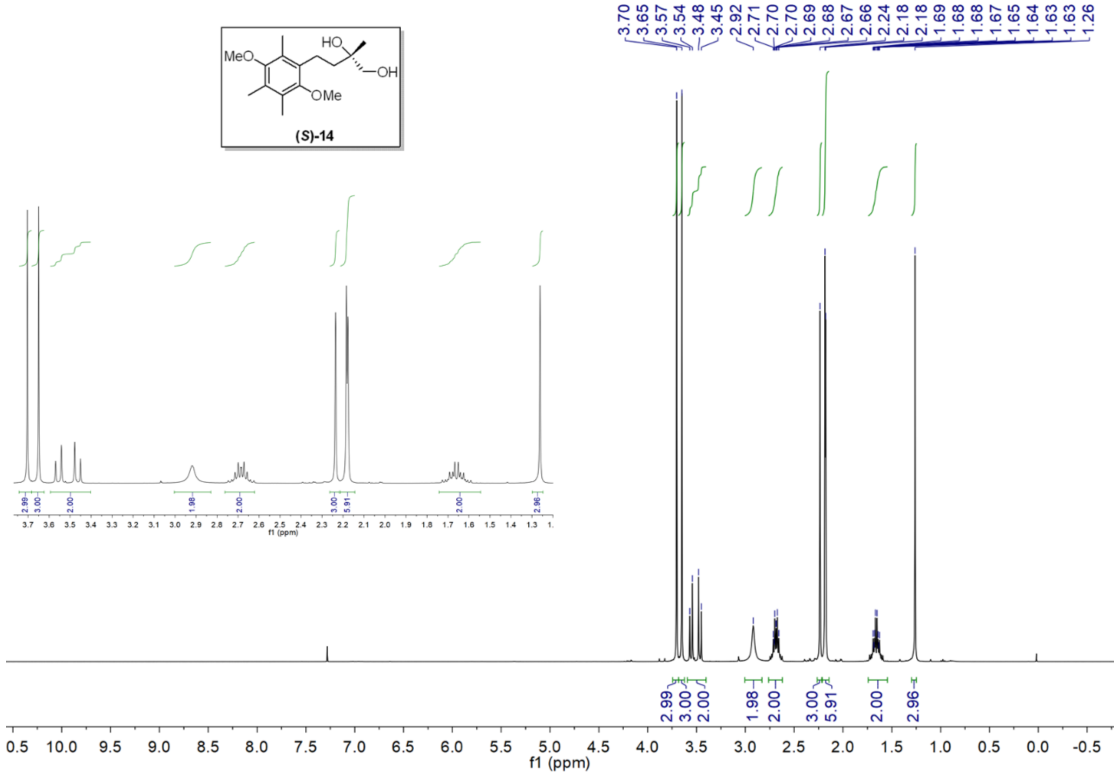
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of (*S*)-50



The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of (*S*)-50



The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of (*S*)-14



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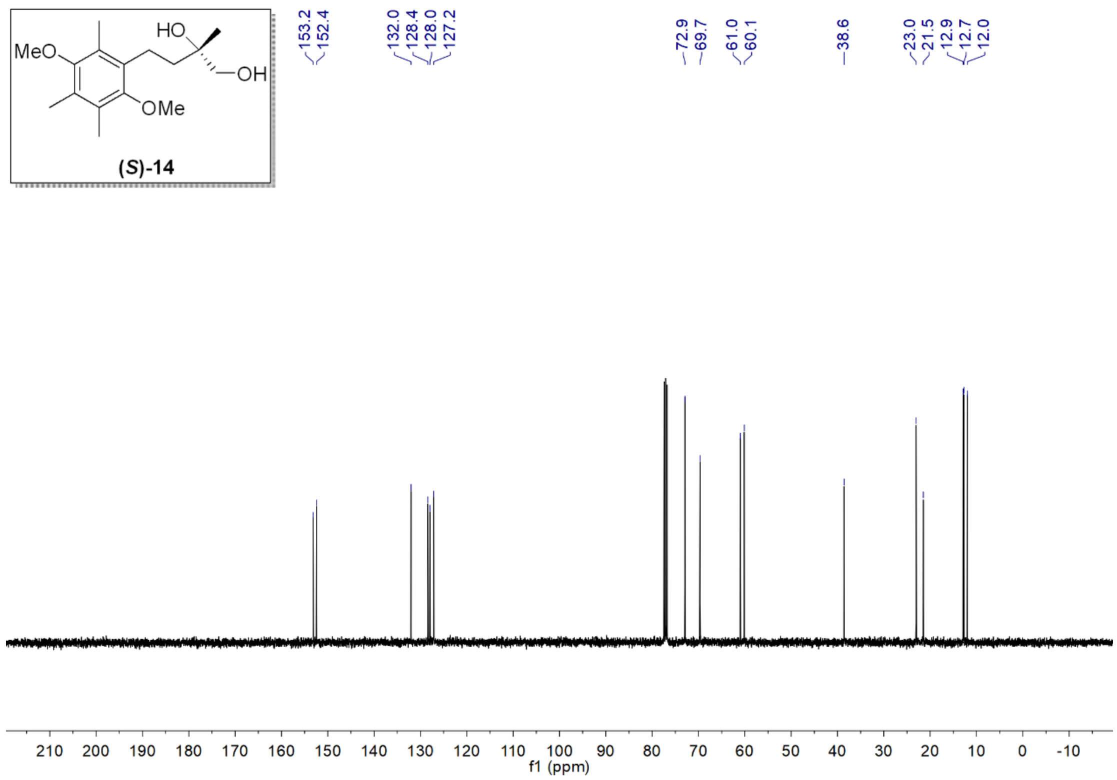
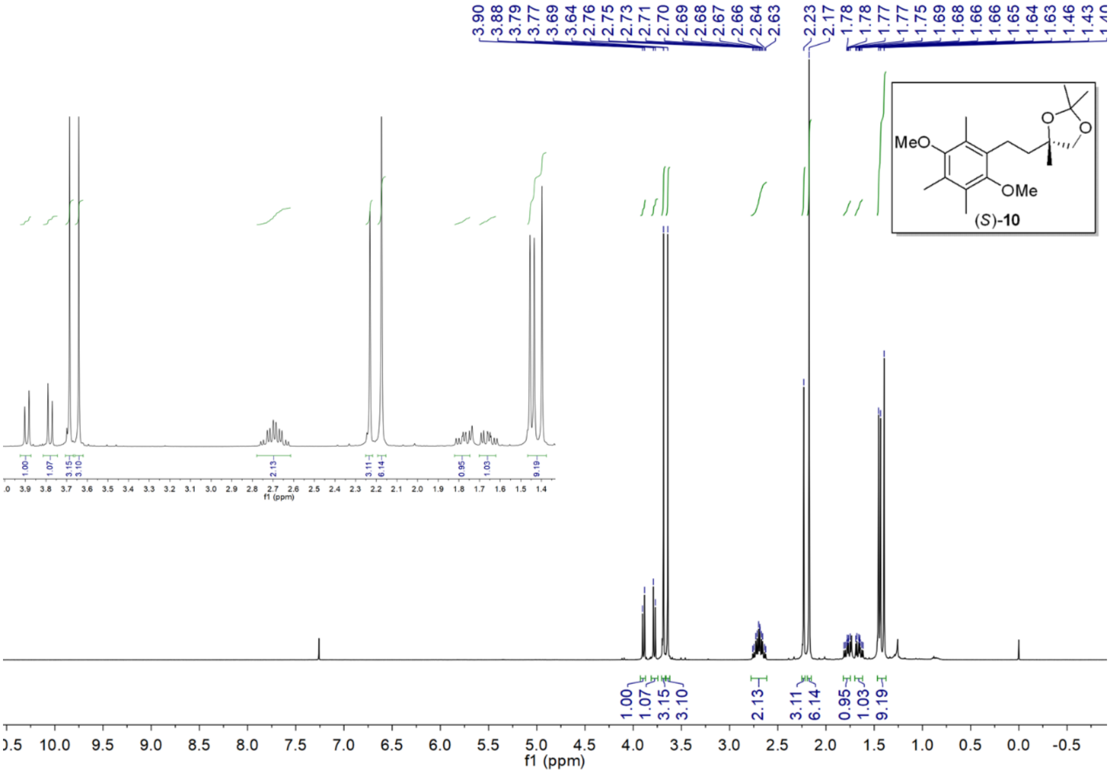


The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of (*S*)-10



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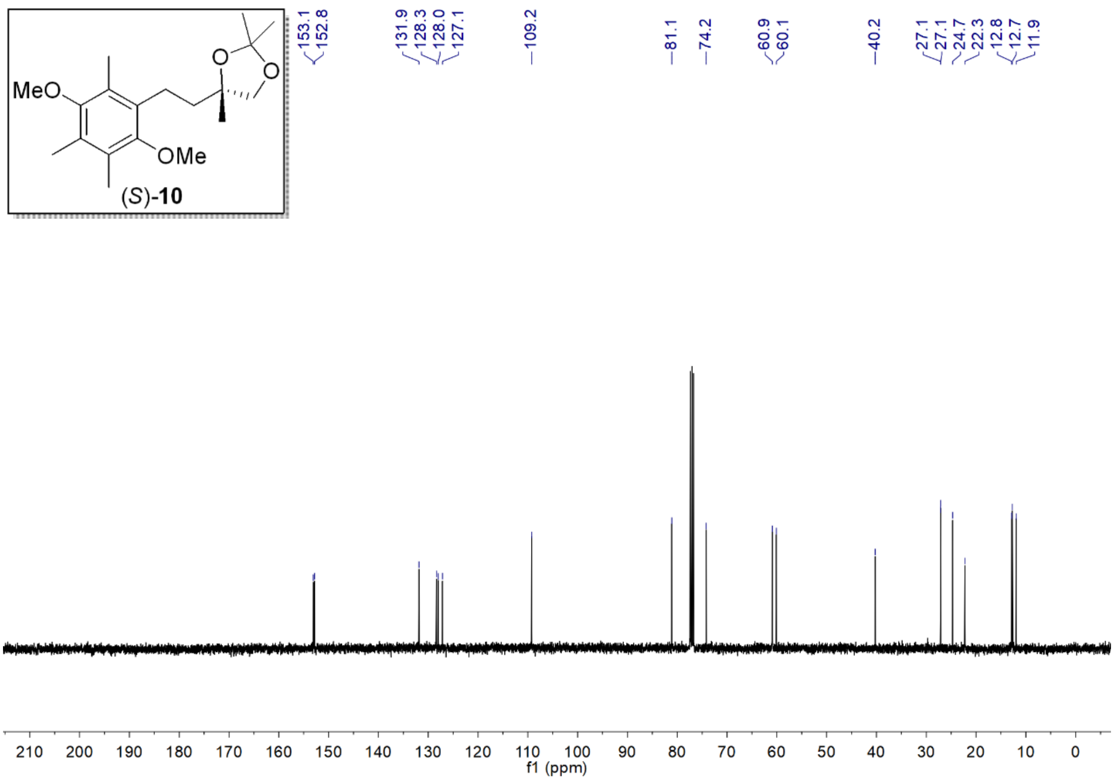

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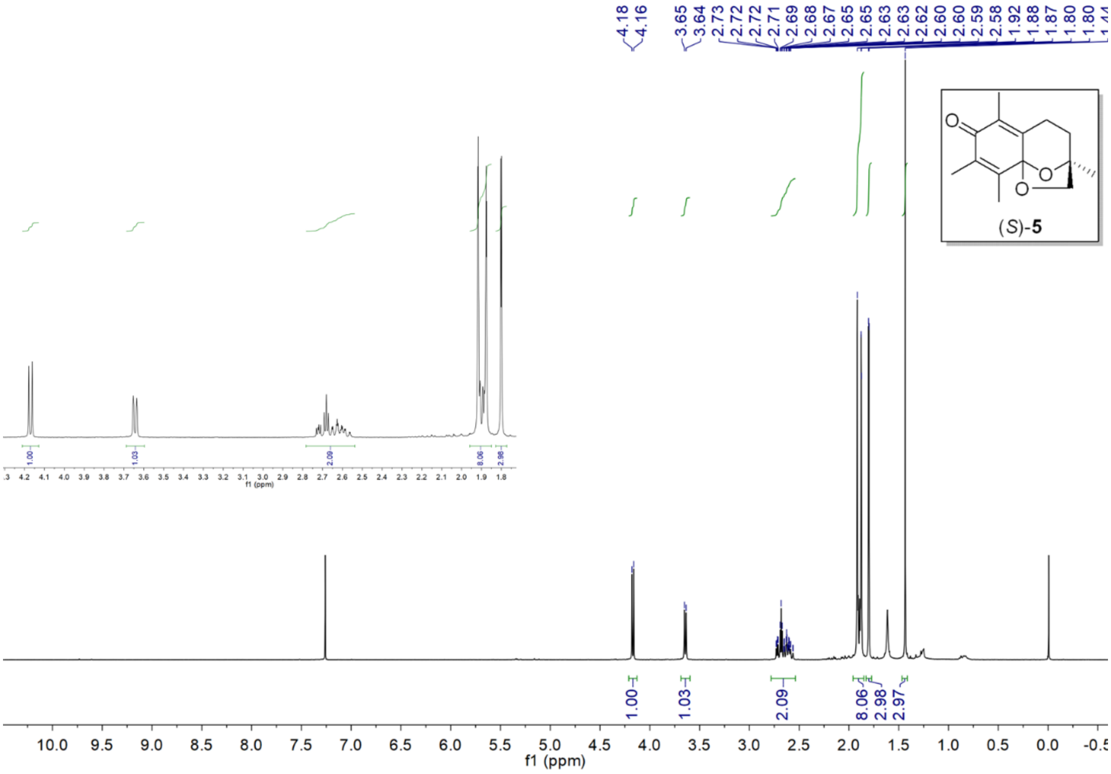
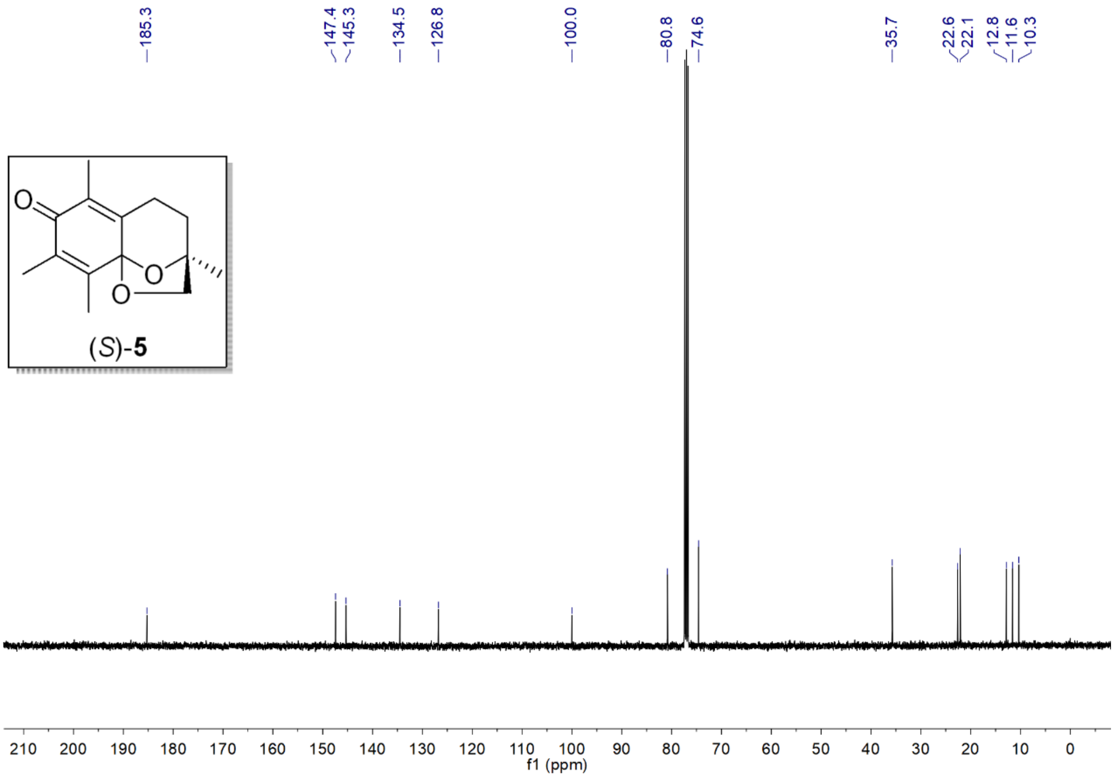
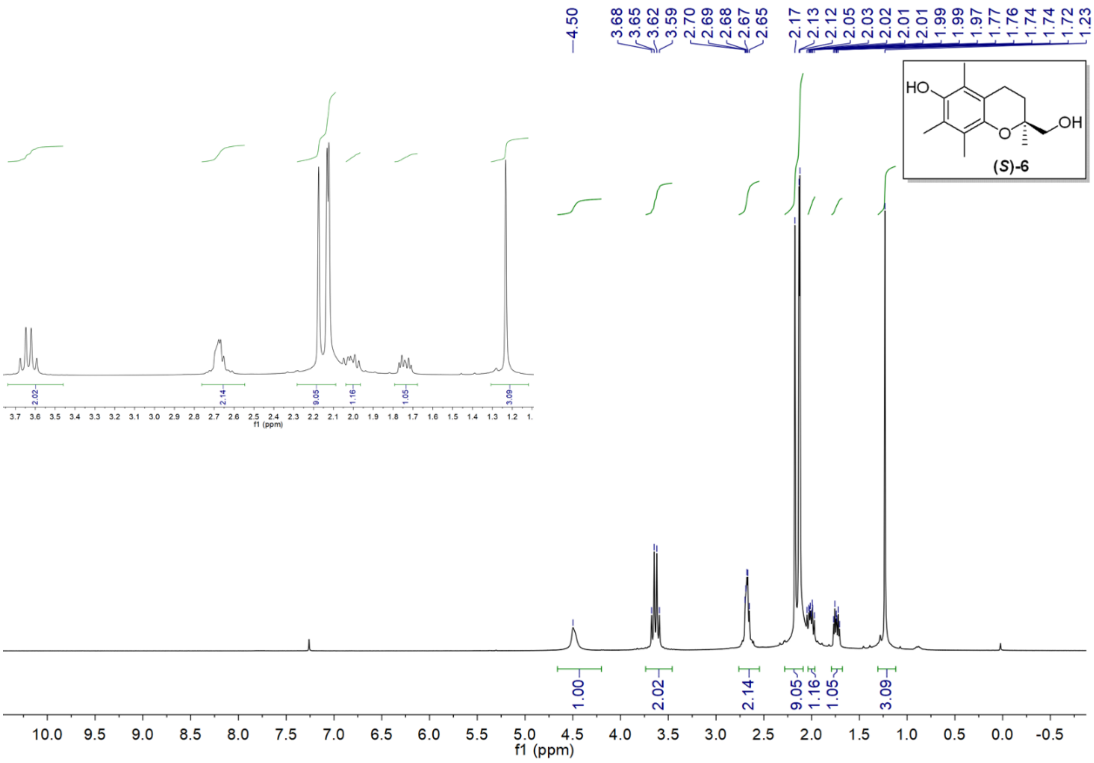


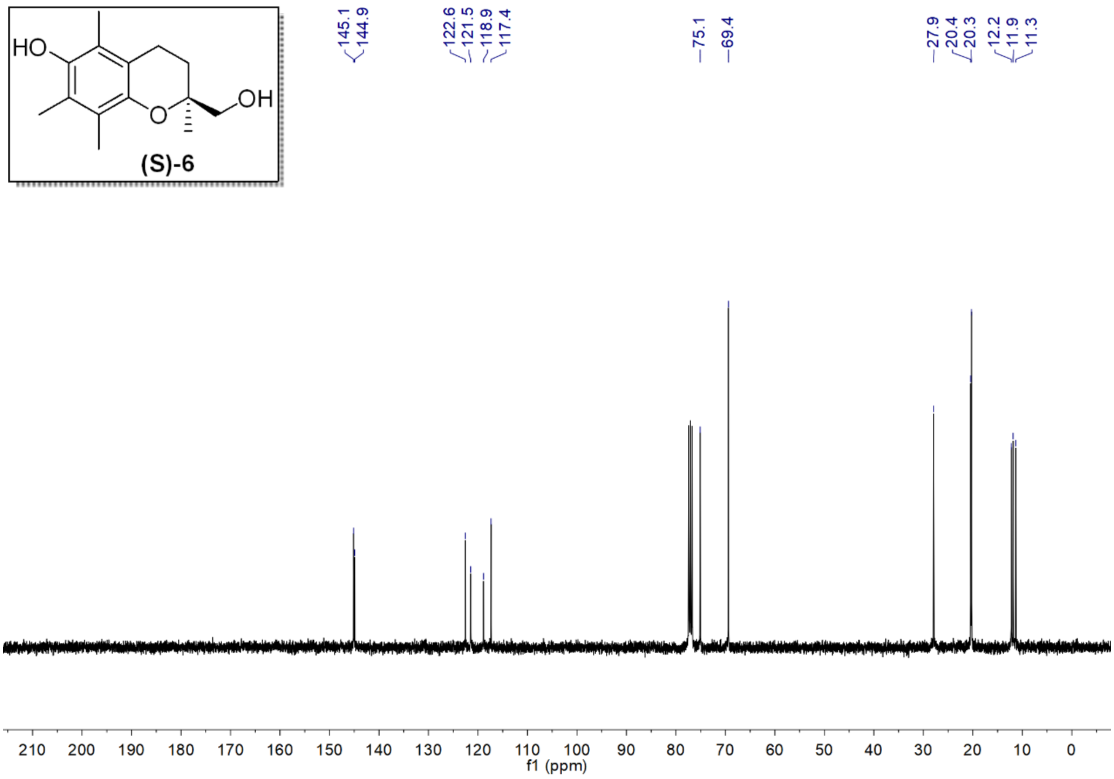
The ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) Spectrum of (*S*)-5



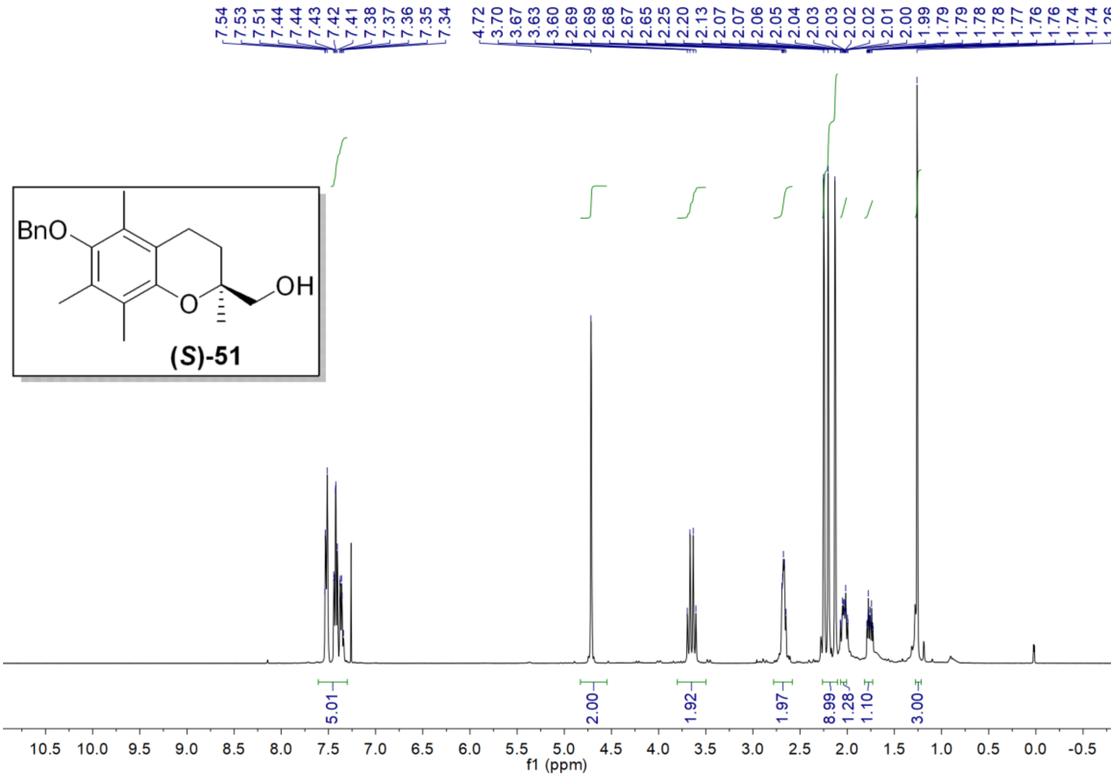
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of (*S*)-6



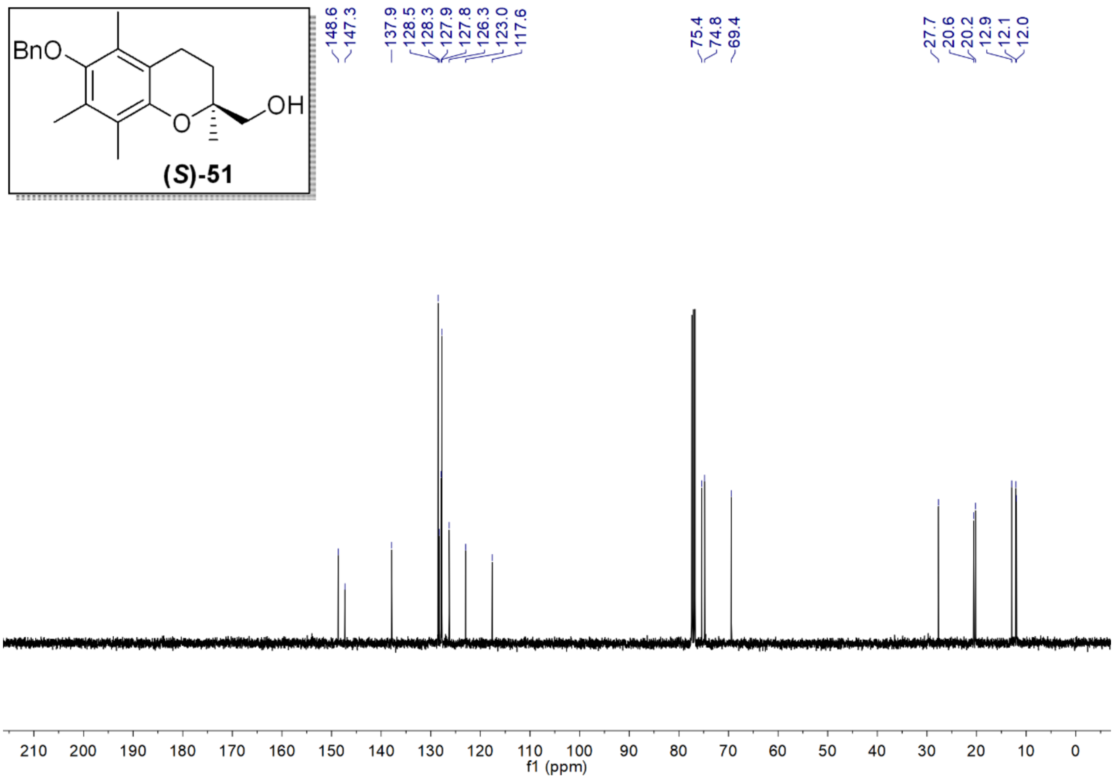
The ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) Spectrum of (*S*)-6



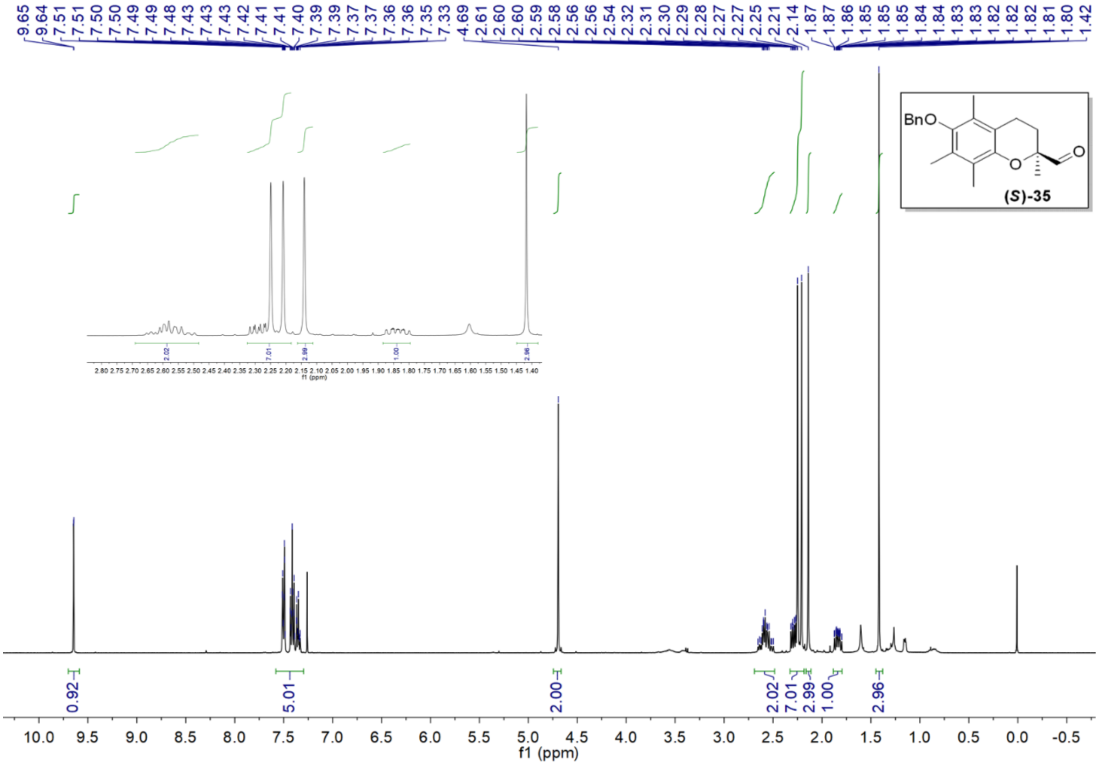
The ^{1}H NMR (400 MHz, CDCl$_3$) Spectrum of (*S*)-51



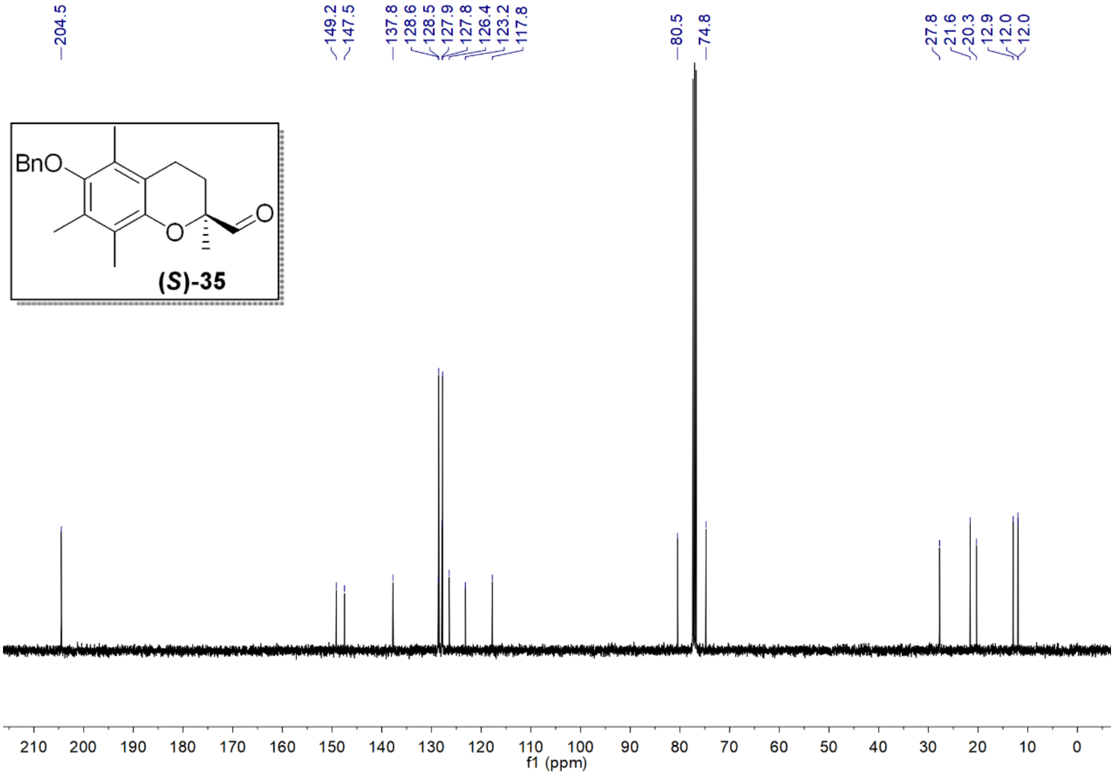
The ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) Spectrum of (*S*)-51



The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of (*S*)-35



The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of (*S*)-35



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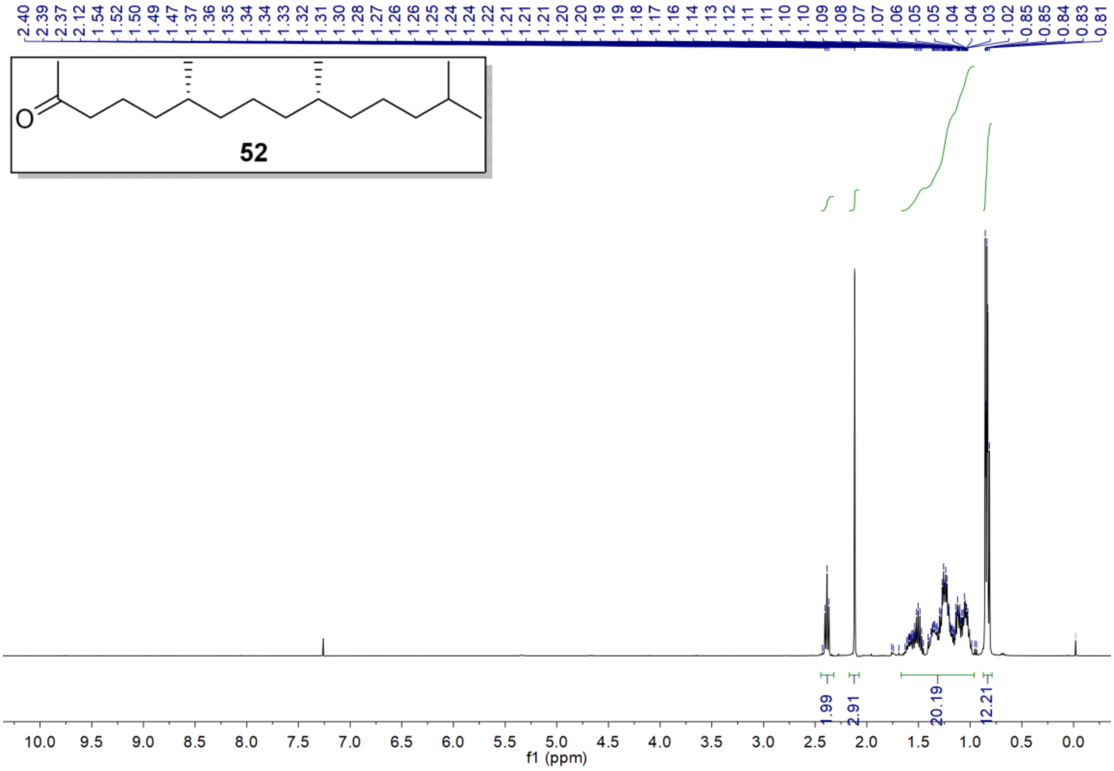
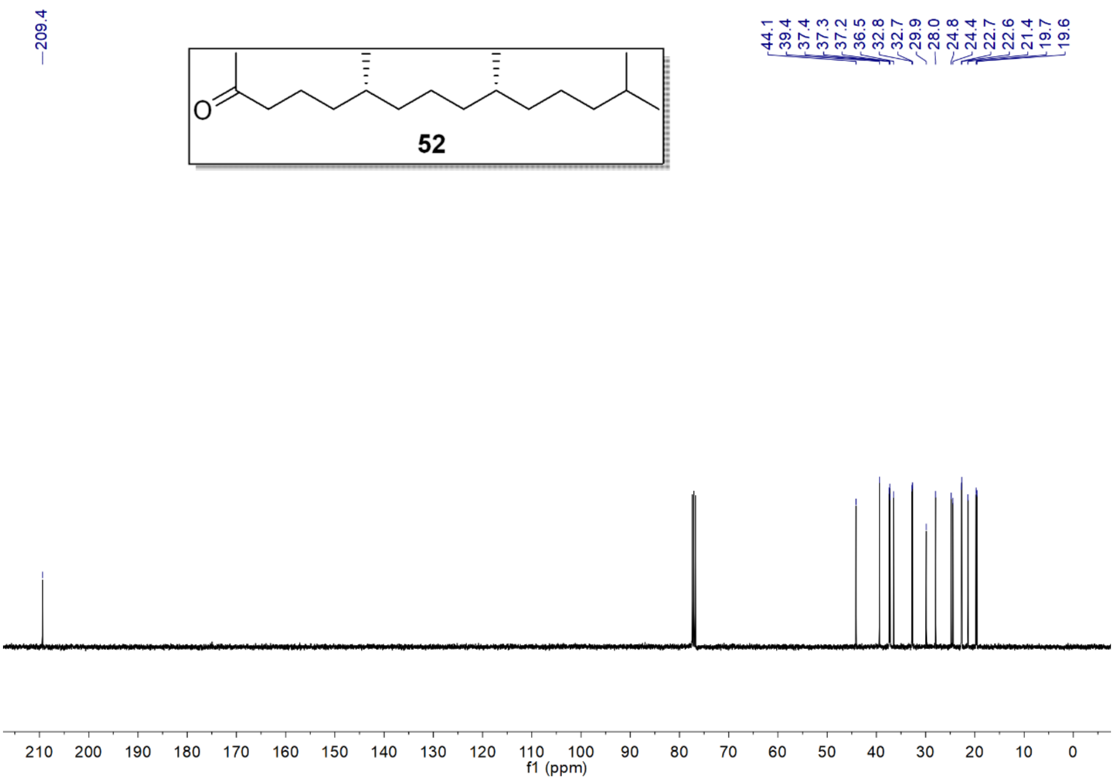
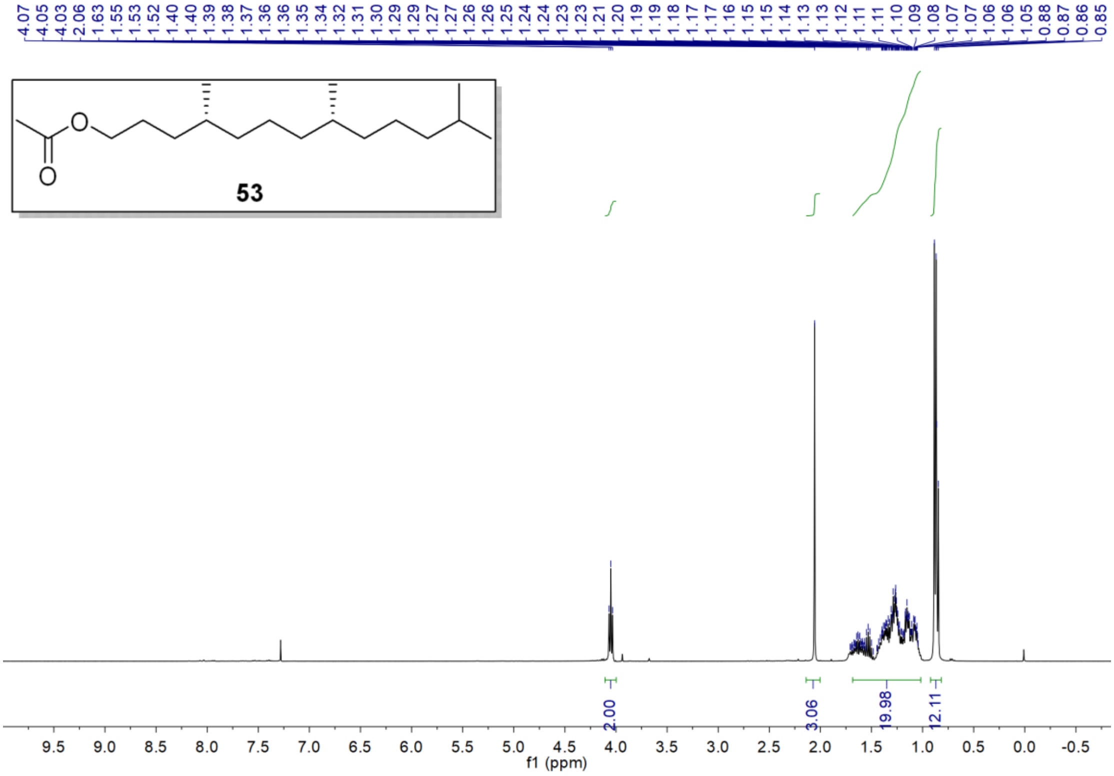


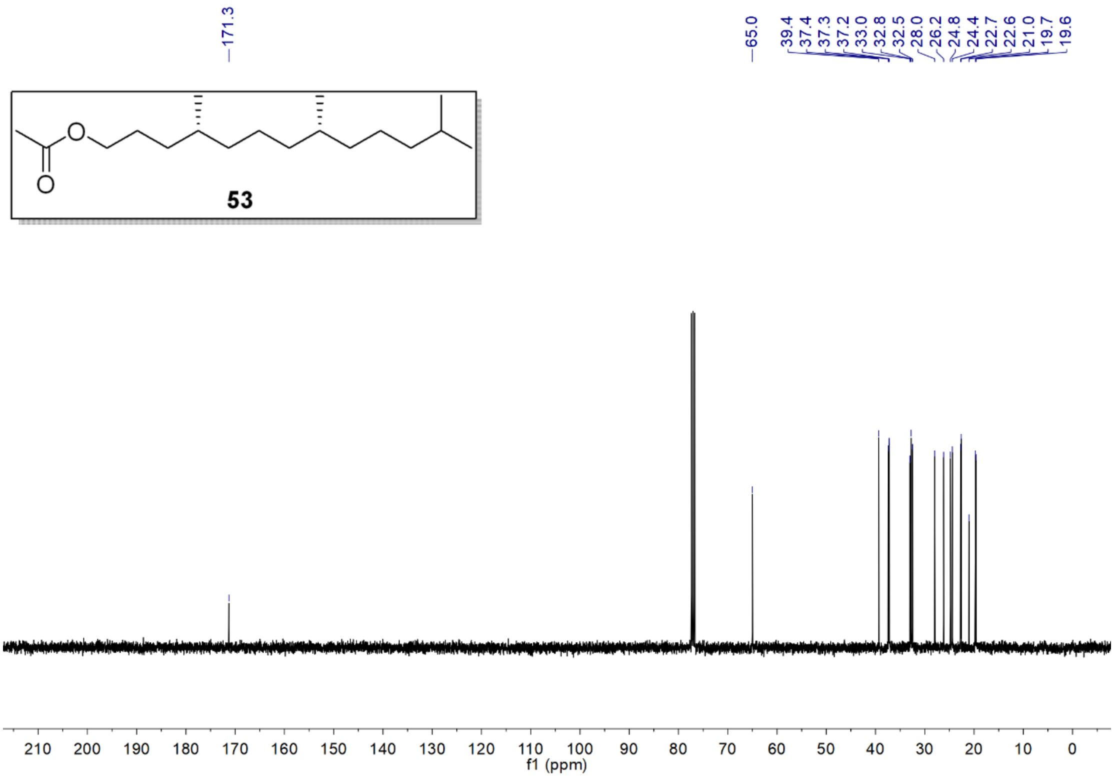
The ¹³C{¹H} NMR (100 MHz, CDCl₃) Spectrum of 52



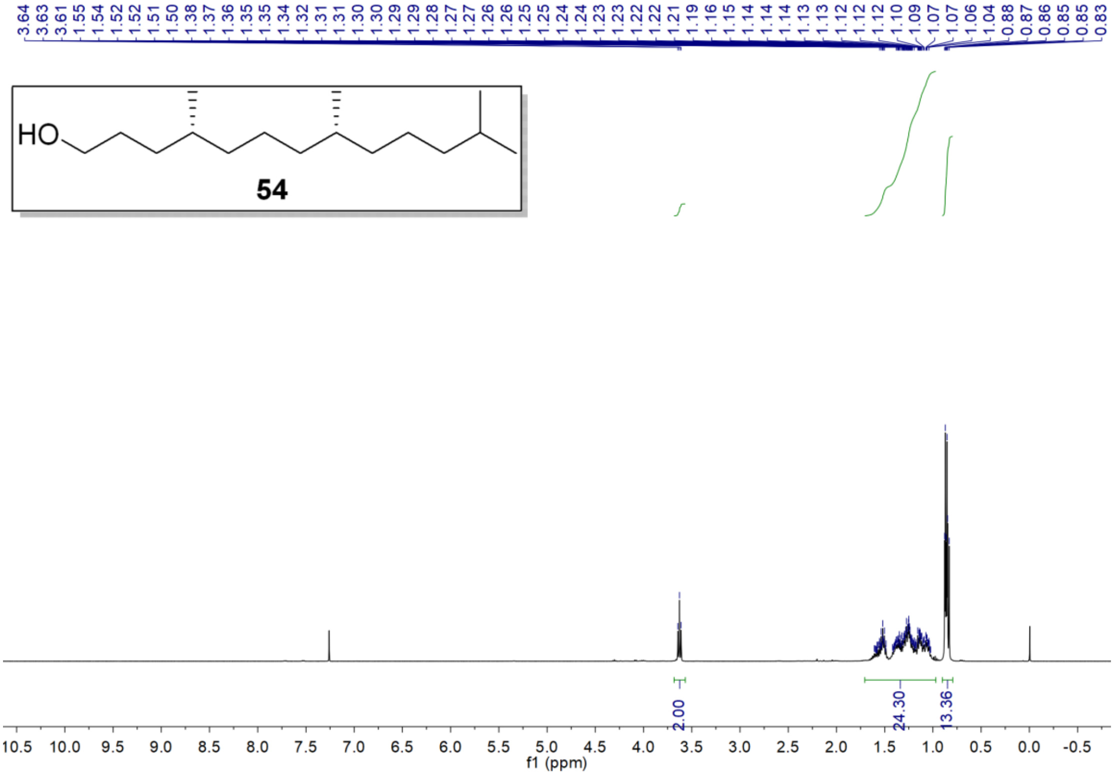
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of 53



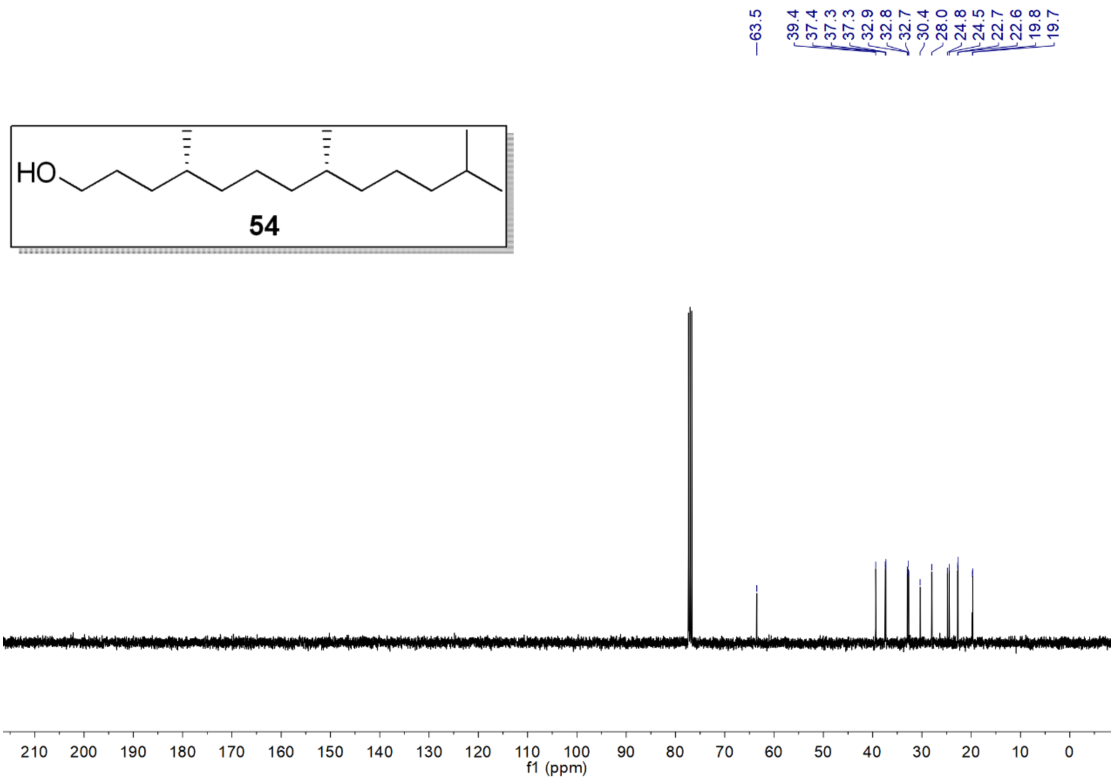
The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of 53



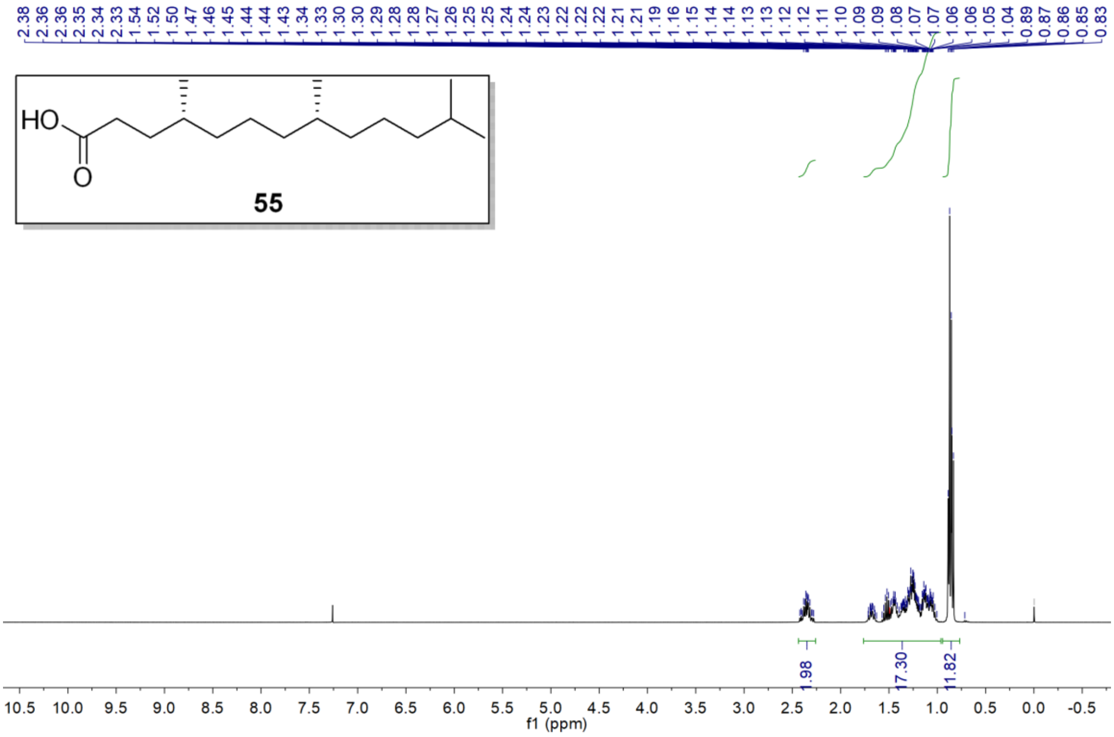
The [1]H NMR (400 MHz, CDCl₃) Spectrum of 54



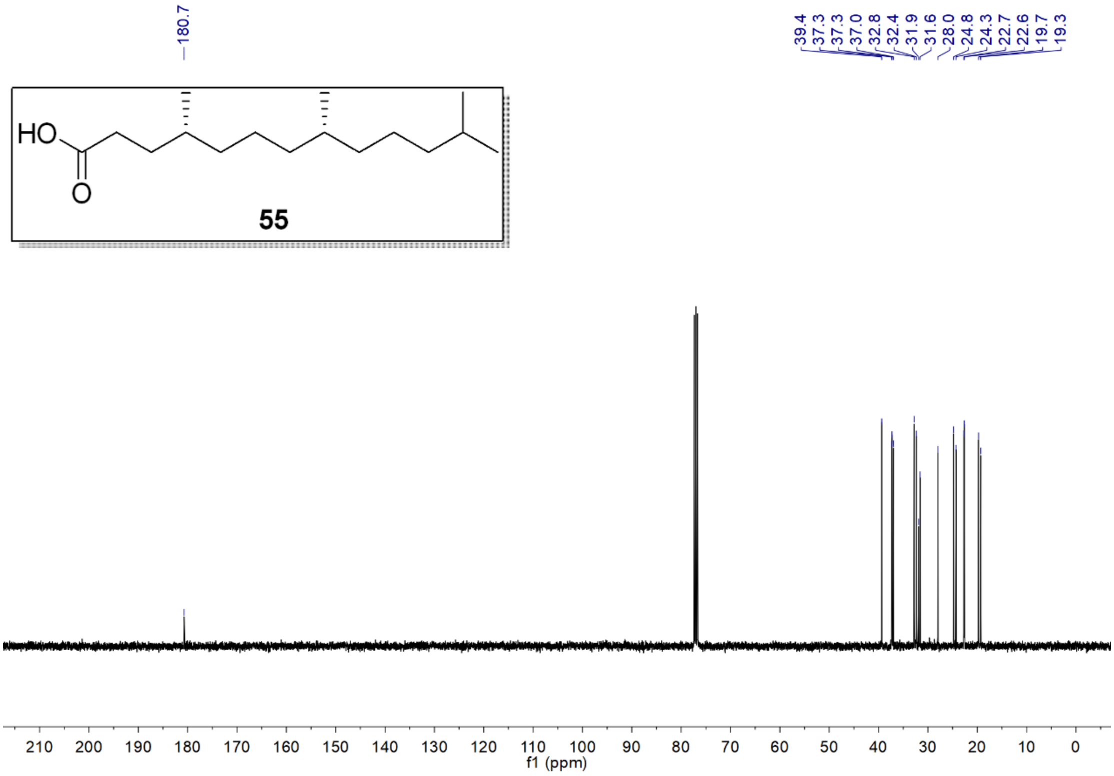
The [13]C{[1]H} NMR (100 MHz, CDCl₃) Spectrum of 54



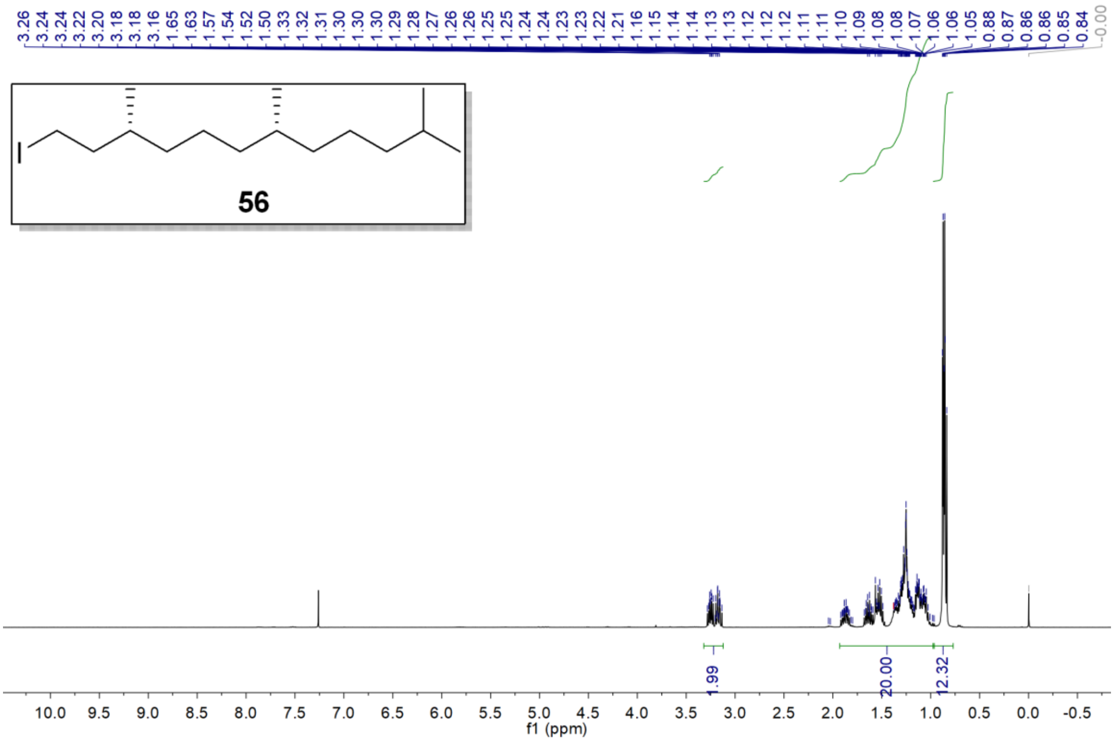
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of 55



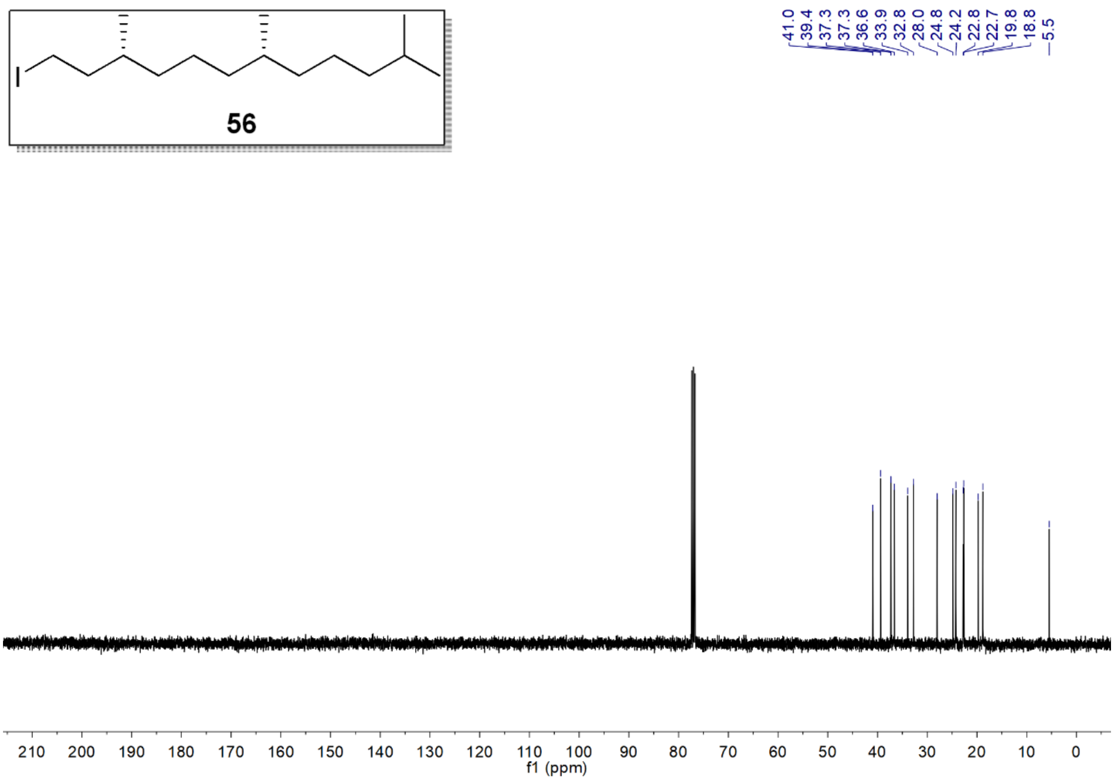
The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of 55



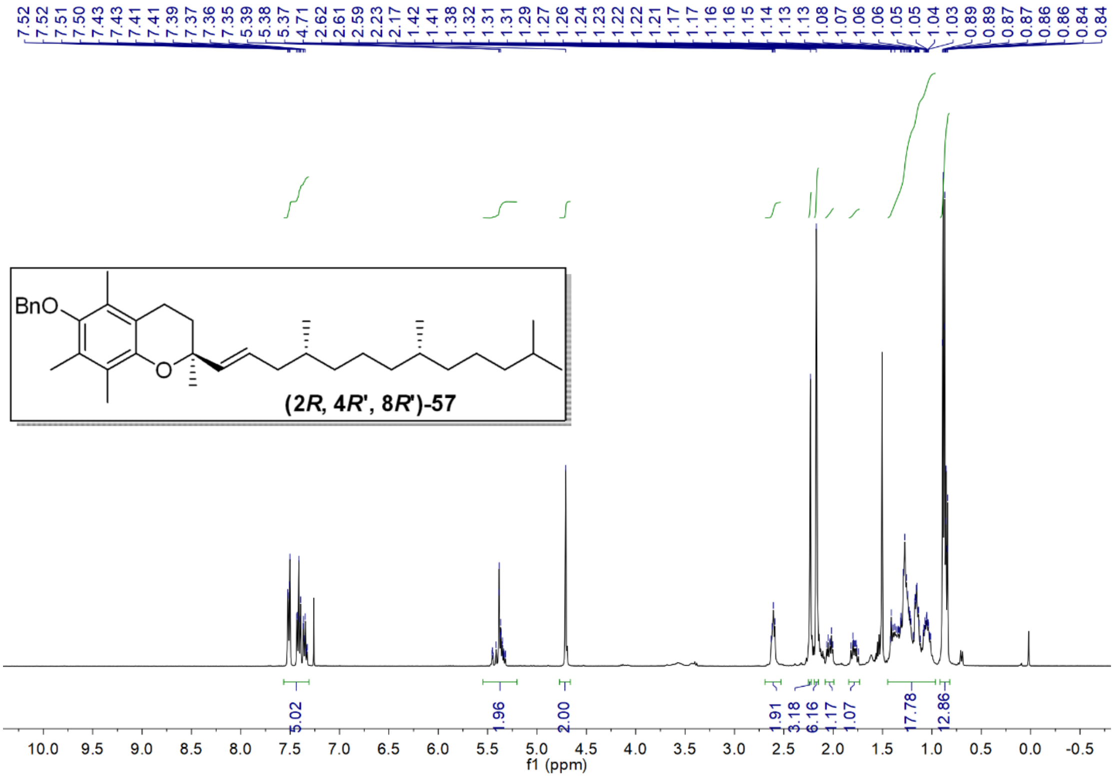
The ¹H NMR (400 MHz, $CDCl_3$) Spectrum of 56



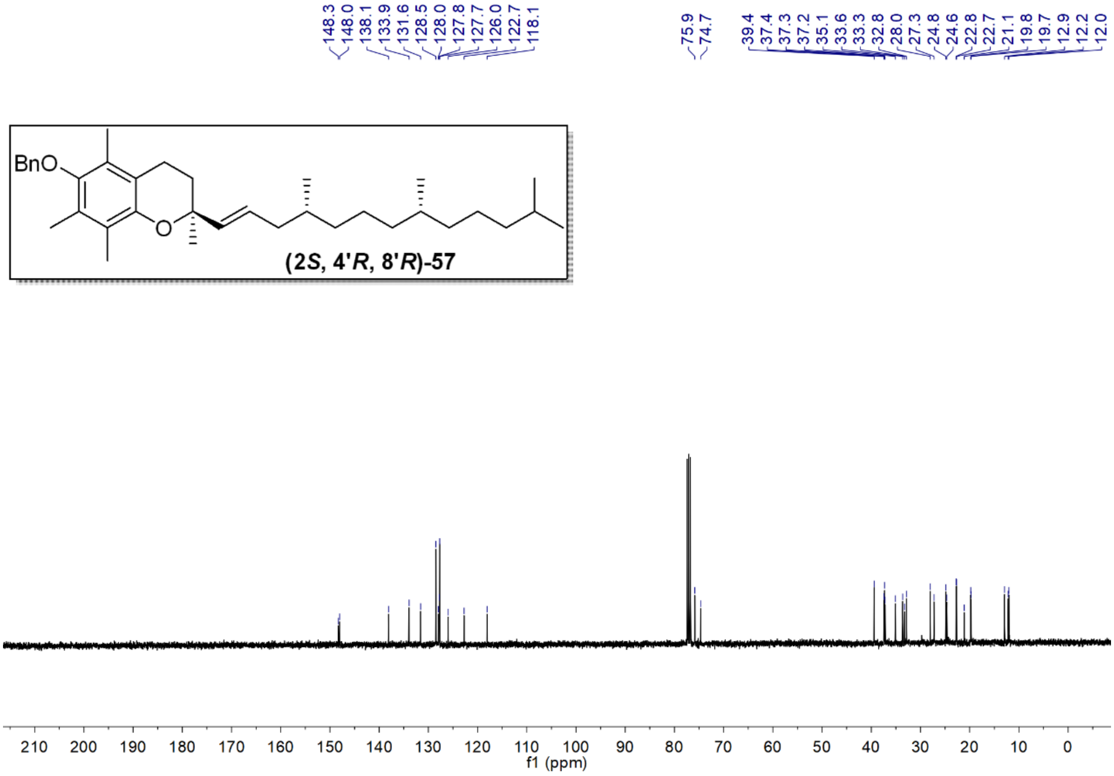
The $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of 56



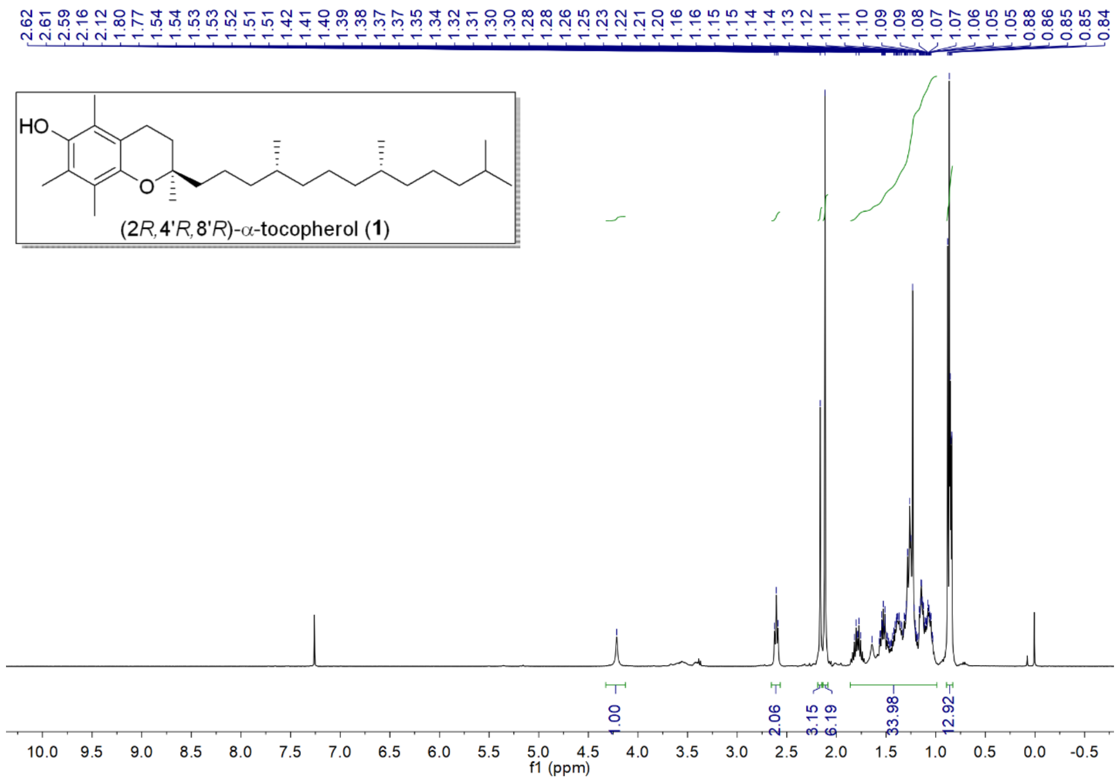
The ¹H NMR (400 MHz, $CDCl_3$) Spectrum of 57



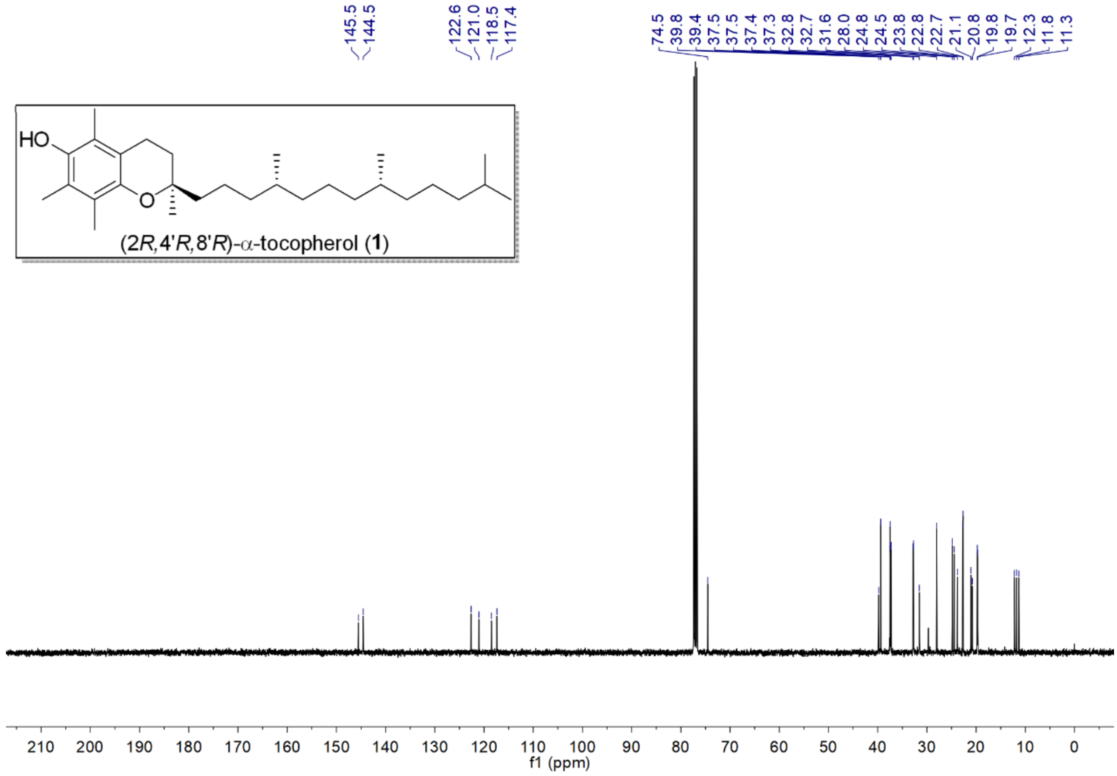
The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of 57



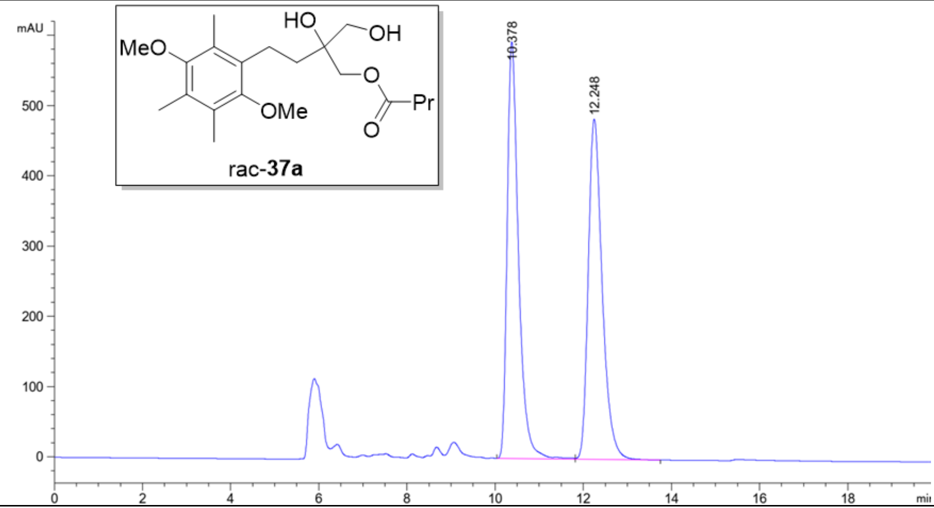
The ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of 1



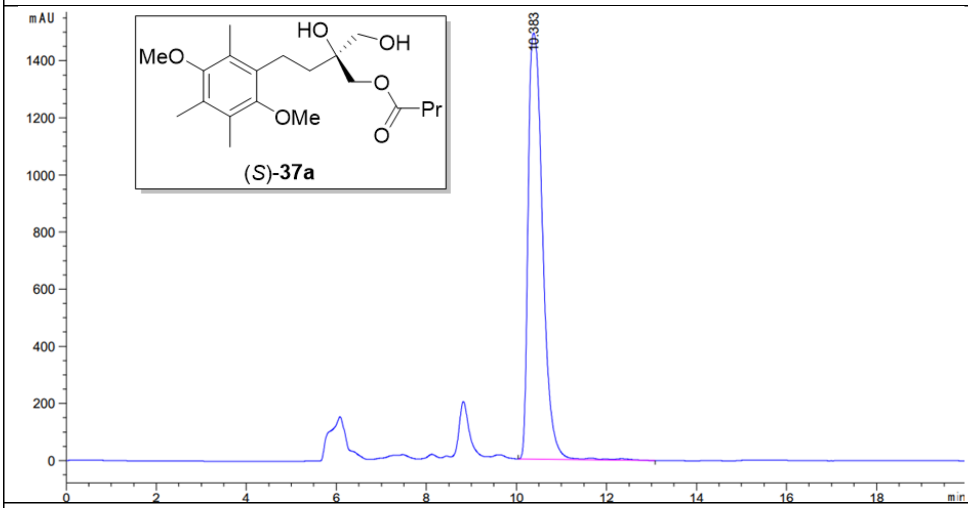
The $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) Spectrum of 1



(*S*)-37a



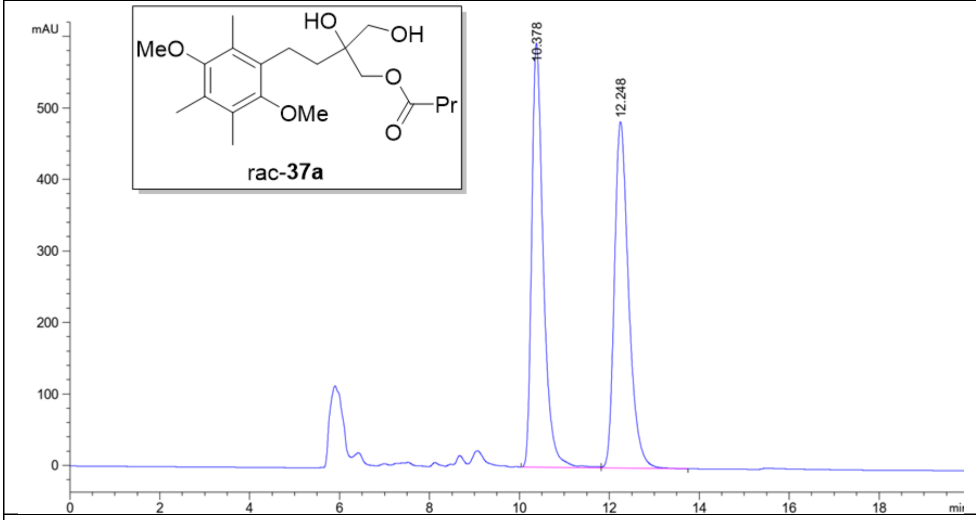
peak # 峰 #	retention time 保留时间 [min]	type 类型	peak width 峰宽 [min]	peak area 峰面积 [mAU*s]	peak height 峰高 [mAU]	peak area 峰面积 %
1	10.378	BV R	0.2715	1.06133e4	592.88495	49.9097
2	12.248	VB	0.3351	1.06517e4	484.48669	50.0903



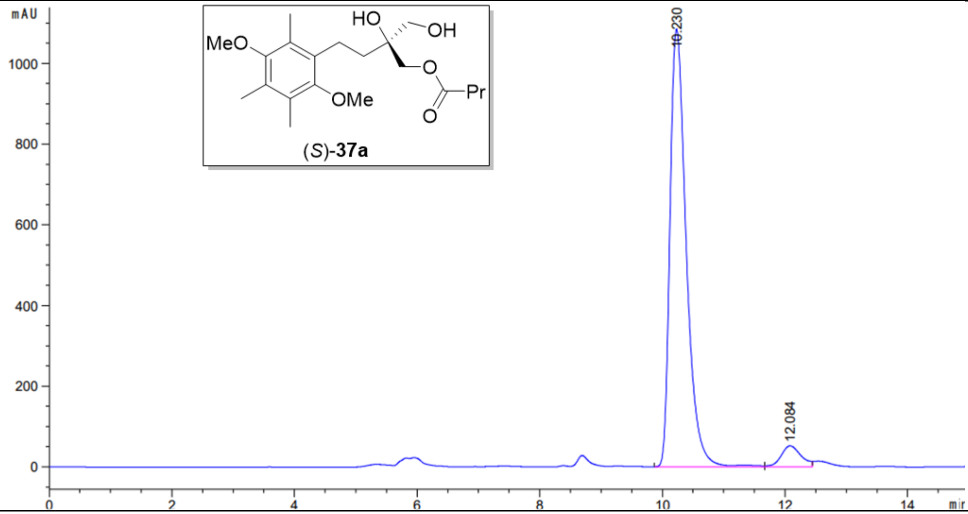
peak # 峰 #	retention time 保留时间 [min]	type 类型	peak width 峰宽 [min]	peak area 峰面积 [mAU*s]	peak height 峰高 [mAU]	peak area 峰面积 %
1	10.383	BV R	0.3496	3.34642e4	1492.62866	100.0000

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of PPL-catalyzed transesterification of triol **38** in analytical scale.

(*S*)-37a



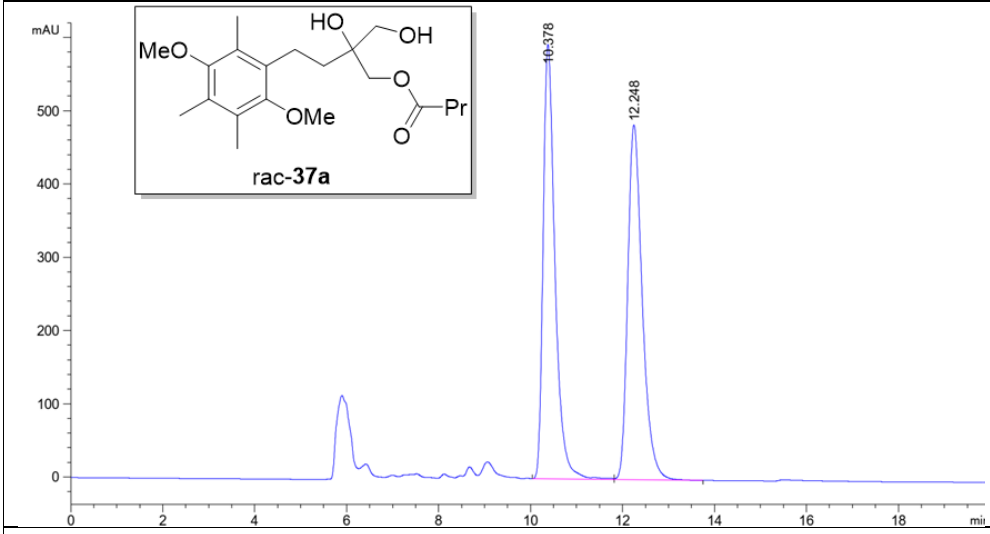
peak 峰 #	retention time 保留时间 [min]	type 类型	peak width 峰宽 [min]	peak area 峰面积 [mAU*s]	peak height 峰高 [mAU]	peak area 峰面积 %
1	10.378	BV R	0.2715	1.06133e4	592.88495	49.9097
2	12.248	VB	0.3351	1.06517e4	484.48669	50.0903



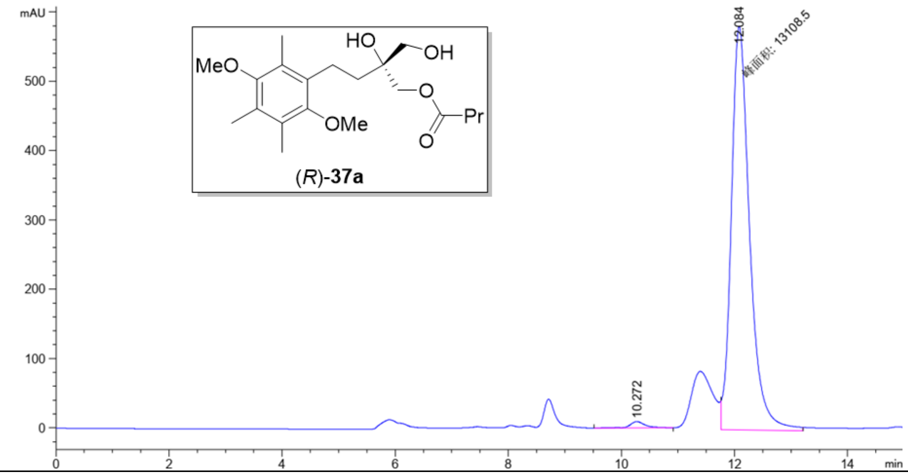
peak 峰 #	retention time 保留时间 [min]	type 类型	peak width 峰宽 [min]	peak area 峰面积 [mAU*s]	peak height 峰高 [mAU]	peak area 峰面积 %
1	10.230	BV R	0.2802	1.99375e4	1084.92773	94.4085
2	12.084	VV	0.3424	1180.82068	52.23682	5.5915

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of PPL-catalyzed transesterification of triol **38** in 200 mg scale.

(*R*)-37a



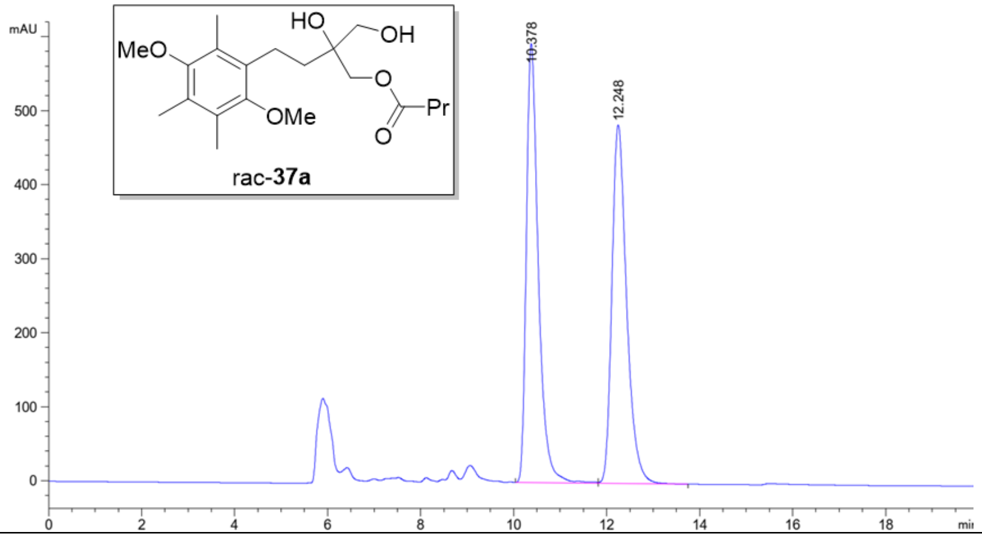
peak 峰 #	retention time 保留时间 [min]	type 类型	peak width 峰宽 [min]	peak area 峰面积 [mAU*s]	peak height 峰高 [mAU]	peak area 峰面积 %
1	10.378	BV R	0.2715	1.06133e4	592.88495	49.9097
2	12.248	VB	0.3351	1.06517e4	484.48669	50.0903



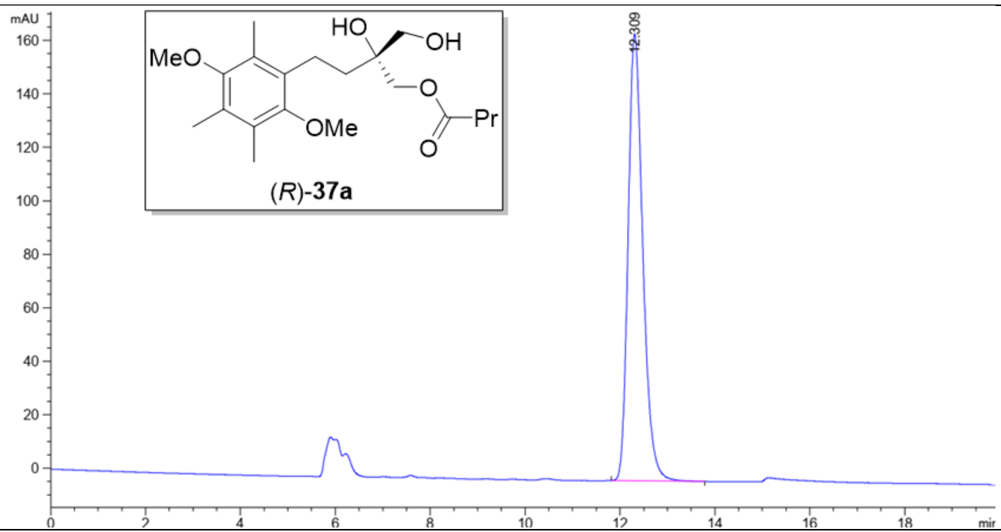
peak 峰 #	retention time 保留时间 [min]	type 类型	peak width 峰宽 [min]	peak area 峰面积 [mAU*s]	peak height 峰高 [mAU]	peak area 峰面积 %
1	10.272	VB R	0.2789	173.52596	9.11401	1.3065
2	12.084	FM	0.3754	1.31085e4	582.03961	98.6935

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of lipase-M-catalyzed hydrolysis of **39a** in analytical scale.

(*R*)-37a



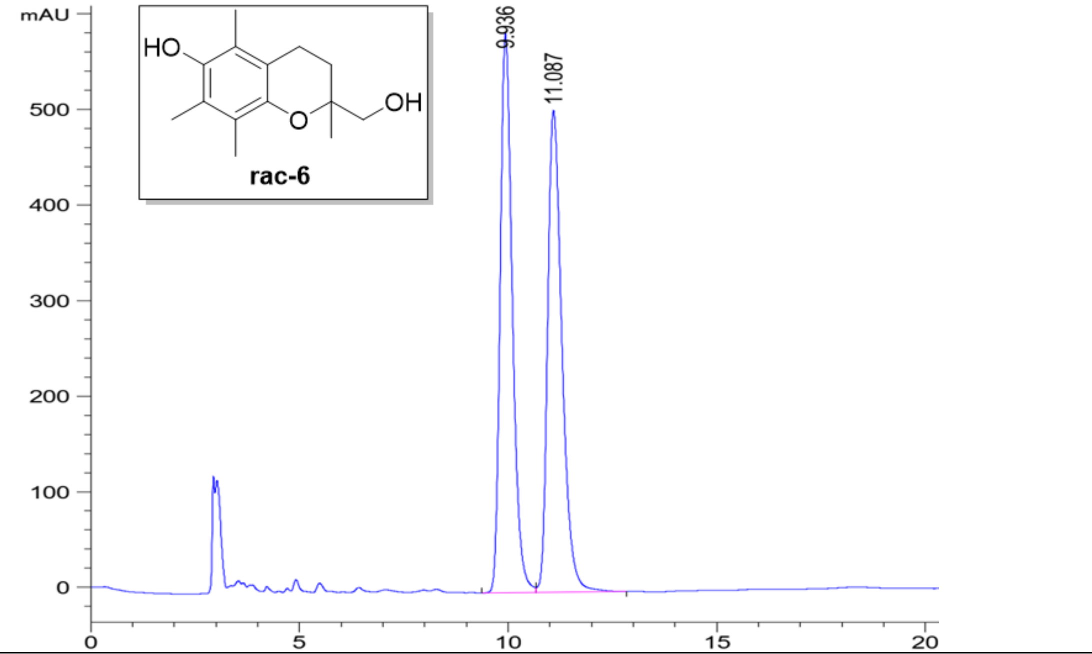
peak 峰 #	retention time 保留时间 [min]	type 类型	peak width 峰宽 [min]	peak area 峰面积 [mAU*s]	peak height 峰高 [mAU]	peak area 峰面积 %
1	10.378	BV R	0.2715	1.06133e4	592.88495	49.9097
2	12.248	VB	0.3351	1.06517e4	484.48669	50.0903



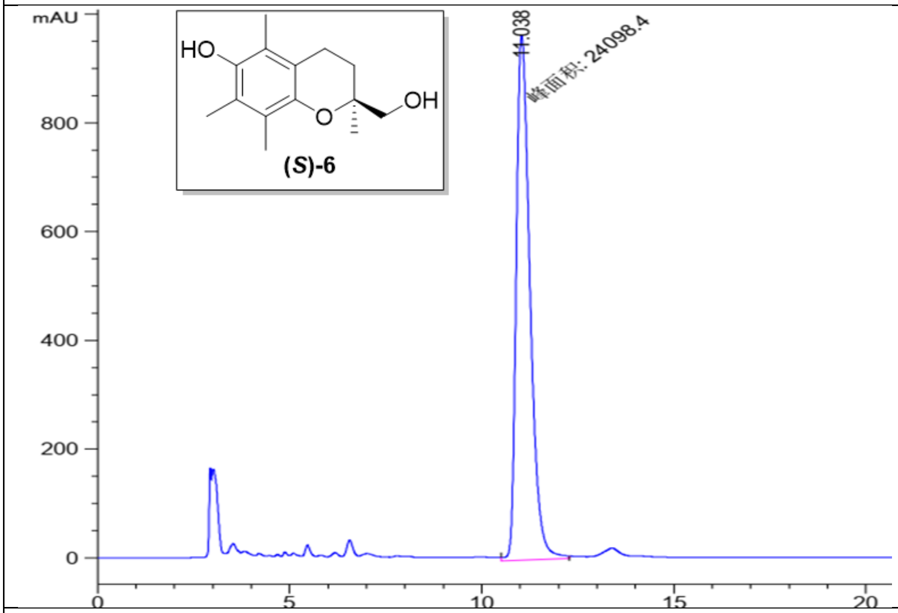
peak 峰 #	retention time 保留时间 [min]	type 类型	peak width 峰宽 [min]	peak area 峰面积 [mAU*s]	peak height 峰高 [mAU]	peak area 峰面积 %
1	12.309	BB	0.3313	3598.36743	167.11610	100.0000

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of lipase-M-catalyzed hydrolysis of **39a** in gram scale, product after recrystallization.

(*S*)-6



peak #	retention time [min]	type	peak width [min]	peak area [mAU*s]	peak height [mAU]	peak area %
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.936	BV	0.3123	1.18639e4	585.00037	49.6303
2	11.087	VB	0.3659	1.20407e4	504.37009	50.3697



peak #	retention time [min]	type	peak width [min]	peak area [mAU*s]	peak height [mAU]	peak area %
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.038	MM	0.4161	2.40984e4	965.28284	100.0000

The top spectrum is the chiral HPLC analysis of the racemic synthetic standard. The bottom spectrum is the chiral HPLC analysis of (*S*)-**6**.

Crystallographic information

The crystal data of compound **(*S*)-6** has been deposited in CCDC with number 2115175.

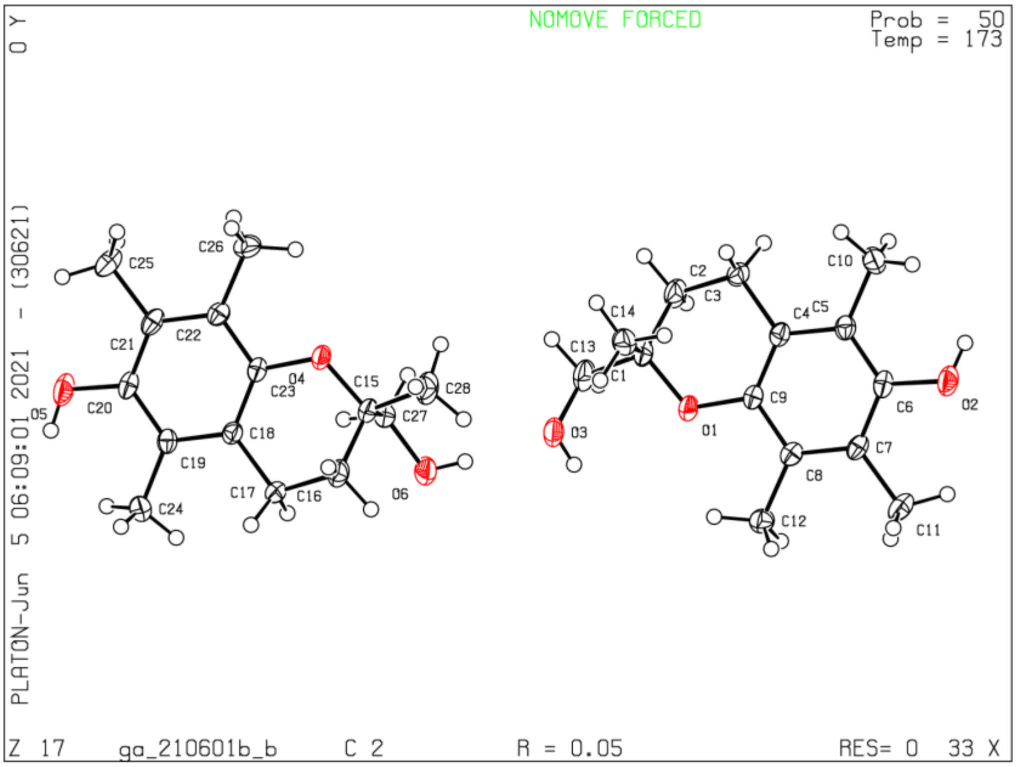


Table 1. Crystal data and structure refinement for CCDC 2115175.

Identification code	ga_210601b_b	
Empirical formula	C14 H20 O3	
Formula weight	236.30	
Temperature	173(2) K	
Wavelength	1.34138 Å	
Crystal system	Monoclinic	
Space group	C2	
Unit cell dimensions	a = 38.9060(12) Å	α= 90°.
	b = 5.7838(2) Å	β= 102.5260(10)°.
	c = 11.1782(3) Å	γ = 90°.
Volume	2455.50(13) Å^3	
Z	8	
Density (calculated)	1.278 Mg/m^3	
Absorption coefficient	0.453 mm^{-1}	
F(000)	1024	
Crystal size	0.430 x 0.290 x 0.010 mm^3	
Theta range for data collection	3.664 to 58.993°.	
Index ranges	-49<=h<=49, -7<=k<=7, -13<=l<=14	
Reflections collected	16142	
Independent reflections	5341 [R(int) = 0.0546]	
Completeness to theta = 53.594°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.752 and 0.579	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5341 / 5 / 331	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)]	R1 = 0.0454, wR2 = 0.1234	
R indices (all data)	R1 = 0.0483, wR2 = 0.1270	
Absolute structure parameter	0.14(12)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.570 and -0.240 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for CCDC 2115175. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5926(1)	6543(3)	7241(1)	26(1)
O(2)	7322(1)	8027(4)	9435(2)	32(1)
O(3)	5238(1)	4918(4)	6471(2)	35(1)
C(1)	5648(1)	7623(4)	7716(2)	26(1)
C(2)	5732(1)	10183(5)	7915(2)	33(1)
C(3)	6076(1)	10529(4)	8857(2)	28(1)
C(4)	6359(1)	8912(4)	8611(2)	21(1)
C(5)	6713(1)	9251(4)	9183(2)	22(1)
C(6)	6968(1)	7804(5)	8881(2)	23(1)
C(7)	6880(1)	6019(4)	8022(2)	22(1)
C(8)	6527(1)	5608(4)	7501(2)	21(1)
C(9)	6269(1)	7062(4)	7806(2)	20(1)
C(10)	6816(1)	11145(5)	10122(2)	30(1)
C(11)	7164(1)	4566(5)	7665(2)	30(1)
C(12)	6421(1)	3682(5)	6592(2)	27(1)
C(13)	5322(1)	7287(5)	6703(2)	35(1)
C(14)	5608(1)	6403(5)	8885(2)	31(1)
O(4)	4049(1)	3411(3)	7868(1)	26(1)
O(5)	2664(1)	1911(4)	5549(2)	35(1)
O(6)	4600(1)	2907(3)	5600(1)	32(1)
C(15)	4332(1)	2418(4)	7390(2)	23(1)
C(16)	4260(1)	-106(5)	7102(2)	29(1)
C(17)	3916(1)	-456(4)	6163(2)	26(1)
C(18)	3627(1)	1096(4)	6419(2)	20(1)
C(19)	3275(1)	733(4)	5818(2)	21(1)
C(20)	3017(1)	2156(4)	6117(2)	22(1)
C(21)	3097(1)	3922(4)	6979(2)	23(1)
C(22)	3449(1)	4351(4)	7528(2)	21(1)
C(23)	3708(1)	2918(4)	7245(2)	20(1)
C(24)	3182(1)	-1128(5)	4866(2)	29(1)
C(25)	2809(1)	5355(5)	7320(2)	32(1)
C(26)	3549(1)	6301(5)	8431(2)	29(1)

C(27)	4355(1)	3830(4)	6251(2)	25(1)
C(28)	4659(1)	2767(6)	8403(2)	37(1)

Table 3. Bond lengths [Å] and angles [°] for CCDC 2115175.

O(1)-C(9)	1.381(2)
O(1)-C(1)	1.444(3)
O(2)-C(6)	1.387(2)
O(2)-H(2)	0.87(3)
O(3)-C(13)	1.419(4)
O(3)-H(3)	0.82(3)
C(1)-C(13)	1.520(3)
C(1)-C(14)	1.522(3)
C(1)-C(2)	1.522(4)
C(2)-C(3)	1.526(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.513(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(9)	1.393(3)
C(4)-C(5)	1.401(3)
C(5)-C(6)	1.395(3)
C(5)-C(10)	1.510(3)
C(6)-C(7)	1.401(3)
C(7)-C(8)	1.391(3)
C(7)-C(11)	1.510(3)
C(8)-C(9)	1.406(3)
C(8)-C(12)	1.504(3)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-H(14A)	0.9800

C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
O(4)-C(23)	1.386(2)
O(4)-C(15)	1.444(2)
O(5)-C(20)	1.387(2)
O(5)-H(5)	0.88(3)
O(6)-C(27)	1.423(3)
O(6)-H(6)	0.84(3)
C(15)-C(16)	1.508(4)
C(15)-C(28)	1.522(3)
C(15)-C(27)	1.530(3)
C(16)-C(17)	1.526(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.513(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(23)	1.392(3)
C(18)-C(19)	1.403(3)
C(19)-C(20)	1.396(3)
C(19)-C(24)	1.502(3)
C(20)-C(21)	1.392(3)
C(21)-C(22)	1.397(3)
C(21)-C(25)	1.509(3)
C(22)-C(23)	1.394(3)
C(22)-C(26)	1.507(3)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-H(28A)	0.9800

C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(9)-O(1)-C(1)	117.63(16)
C(6)-O(2)-H(2)	111(3)
C(13)-O(3)-H(3)	108(2)
O(1)-C(1)-C(13)	103.94(18)
O(1)-C(1)-C(14)	109.79(19)
C(13)-C(1)-C(14)	110.8(2)
O(1)-C(1)-C(2)	108.73(19)
C(13)-C(1)-C(2)	110.6(2)
C(14)-C(1)-C(2)	112.6(2)
C(1)-C(2)-C(3)	110.9(2)
C(1)-C(2)-H(2A)	109.5
C(3)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
C(3)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	108.1
C(4)-C(3)-C(2)	110.9(2)
C(4)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.1
C(9)-C(4)-C(5)	119.07(19)
C(9)-C(4)-C(3)	120.17(18)
C(5)-C(4)-C(3)	120.8(2)
C(6)-C(5)-C(4)	119.1(2)
C(6)-C(5)-C(10)	120.51(19)
C(4)-C(5)-C(10)	120.4(2)
O(2)-C(6)-C(5)	121.7(2)
O(2)-C(6)-C(7)	116.52(19)
C(5)-C(6)-C(7)	121.77(18)
C(8)-C(7)-C(6)	119.09(19)
C(8)-C(7)-C(11)	120.5(2)
C(6)-C(7)-C(11)	120.44(19)
C(7)-C(8)-C(9)	119.2(2)
C(7)-C(8)-C(12)	120.73(19)

C(9)-C(8)-C(12)	120.09(18)
O(1)-C(9)-C(4)	122.95(18)
O(1)-C(9)-C(8)	115.41(19)
C(4)-C(9)-C(8)	121.63(18)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(8)-C(12)-H(12A)	109.5
C(8)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(8)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
O(3)-C(13)-C(1)	112.4(2)
O(3)-C(13)-H(13A)	109.1
C(1)-C(13)-H(13A)	109.1
O(3)-C(13)-H(13B)	109.1
C(1)-C(13)-H(13B)	109.1
H(13A)-C(13)-H(13B)	107.9
C(1)-C(14)-H(14A)	109.5
C(1)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(1)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(23)-O(4)-C(15)	117.06(15)
C(20)-O(5)-H(5)	109(2)
C(27)-O(6)-H(6)	109(3)
O(4)-C(15)-C(16)	110.04(19)

O(4)-C(15)-C(28)	104.65(18)
C(16)-C(15)-C(28)	112.0(2)
O(4)-C(15)-C(27)	106.34(17)
C(16)-C(15)-C(27)	112.39(19)
C(28)-C(15)-C(27)	111.0(2)
C(15)-C(16)-C(17)	111.7(2)
C(15)-C(16)-H(16A)	109.3
C(17)-C(16)-H(16A)	109.3
C(15)-C(16)-H(16B)	109.3
C(17)-C(16)-H(16B)	109.3
H(16A)-C(16)-H(16B)	107.9
C(18)-C(17)-C(16)	111.63(19)
C(18)-C(17)-H(17A)	109.3
C(16)-C(17)-H(17A)	109.3
C(18)-C(17)-H(17B)	109.3
C(16)-C(17)-H(17B)	109.3
H(17A)-C(17)-H(17B)	108.0
C(23)-C(18)-C(19)	119.29(19)
C(23)-C(18)-C(17)	120.21(17)
C(19)-C(18)-C(17)	120.5(2)
C(20)-C(19)-C(18)	118.4(2)
C(20)-C(19)-C(24)	121.12(18)
C(18)-C(19)-C(24)	120.44(19)
O(5)-C(20)-C(21)	116.33(19)
O(5)-C(20)-C(19)	121.5(2)
C(21)-C(20)-C(19)	122.16(18)
C(20)-C(21)-C(22)	119.14(19)
C(20)-C(21)-C(25)	120.64(19)
C(22)-C(21)-C(25)	120.2(2)
C(23)-C(22)-C(21)	118.9(2)
C(23)-C(22)-C(26)	120.15(19)
C(21)-C(22)-C(26)	120.92(19)
O(4)-C(23)-C(18)	122.98(18)
O(4)-C(23)-C(22)	115.07(19)
C(18)-C(23)-C(22)	121.93(18)
C(19)-C(24)-H(24A)	109.5
C(19)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5

C(19)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(21)-C(25)-H(25A)	109.5
C(21)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(21)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(22)-C(26)-H(26A)	109.5
C(22)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(22)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
O(6)-C(27)-C(15)	112.99(18)
O(6)-C(27)-H(27A)	109.0
C(15)-C(27)-H(27A)	109.0
O(6)-C(27)-H(27B)	109.0
C(15)-C(27)-H(27B)	109.0
H(27A)-C(27)-H(27B)	107.8
C(15)-C(28)-H(28A)	109.5
C(15)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(15)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for CCDC 2115175. 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)	14(1)	33(1)	29(1)	-4(1)	2(1)	1(1)
O(2)	15(1)	50(1)	30(1)	-4(1)	1(1)	1(1)
O(3)	18(1)	52(1)	35(1)	-12(1)	6(1)	-6(1)
C(1)	14(1)	29(1)	33(1)	-1(1)	5(1)	1(1)
C(2)	19(1)	27(1)	53(1)	2(1)	5(1)	5(1)
C(3)	21(1)	20(1)	44(1)	-2(1)	9(1)	1(1)
C(4)	18(1)	21(1)	24(1)	4(1)	7(1)	1(1)
C(5)	19(1)	25(1)	22(1)	2(1)	7(1)	-3(1)
C(6)	16(1)	34(1)	18(1)	4(1)	4(1)	-1(1)
C(7)	18(1)	29(1)	18(1)	4(1)	7(1)	4(1)
C(8)	20(1)	25(1)	17(1)	4(1)	5(1)	3(1)
C(9)	16(1)	24(1)	20(1)	3(1)	4(1)	1(1)
C(10)	27(1)	34(1)	31(1)	-6(1)	7(1)	-8(1)
C(11)	22(1)	43(2)	27(1)	1(1)	7(1)	10(1)
C(12)	25(1)	33(1)	24(1)	-4(1)	5(1)	1(1)
C(13)	17(1)	45(2)	41(1)	0(1)	0(1)	3(1)
C(14)	28(1)	31(1)	34(1)	-4(1)	10(1)	-7(1)
O(4)	14(1)	38(1)	27(1)	-9(1)	4(1)	-1(1)
O(5)	15(1)	58(1)	31(1)	-3(1)	2(1)	2(1)
O(6)	23(1)	42(1)	34(1)	-6(1)	11(1)	-8(1)
C(15)	14(1)	28(1)	28(1)	-2(1)	4(1)	2(1)
C(16)	18(1)	24(1)	45(1)	4(1)	7(1)	2(1)
C(17)	18(1)	22(1)	39(1)	-7(1)	9(1)	1(1)
C(18)	18(1)	21(1)	23(1)	1(1)	7(1)	0(1)
C(19)	18(1)	24(1)	22(1)	2(1)	6(1)	-3(1)
C(20)	15(1)	34(1)	19(1)	6(1)	4(1)	3(1)
C(21)	19(1)	33(1)	19(1)	7(1)	7(1)	6(1)
C(22)	21(1)	26(1)	16(1)	2(1)	7(1)	2(1)
C(23)	16(1)	26(1)	19(1)	2(1)	5(1)	1(1)
C(24)	23(1)	32(1)	34(1)	-7(1)	8(1)	-7(1)
C(25)	25(1)	44(2)	28(1)	1(1)	9(1)	12(1)
C(26)	31(1)	33(1)	26(1)	-6(1)	10(1)	2(1)
C(27)	19(1)	24(1)	33(1)	-3(1)	6(1)	-1(1)

C(28)	18(1)	54(2)	36(1)	-3(1)	-2(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for CCDC 2115175.

	x	y	z	U(eq)
H(2)	7368(10)	9410(60)	9720(30)	63(12)
H(3)	5361(8)	4410(60)	6030(30)	40(8)
H(2A)	5538	10958	8202	40
H(2B)	5752	10900	7128	40
H(3A)	6156	12149	8825	34
H(3B)	6036	10238	9689	34
H(10A)	6832	12617	9703	46
H(10B)	7045	10778	10652	46
H(10C)	6638	11270	10619	46
H(11A)	7389	5389	7877	46
H(11B)	7103	4276	6780	46
H(11C)	7183	3090	8105	46
H(12A)	6164	3513	6408	41
H(12B)	6530	2235	6939	41
H(12C)	6499	4042	5837	41
H(13A)	5120	8072	6936	42
H(13B)	5360	8019	5942	42
H(14A)	5532	4805	8694	46
H(14B)	5432	7213	9236	46
H(14C)	5835	6407	9476	46
H(5)	2636(10)	580(60)	5170(30)	66(13)
H(6)	4805(8)	3340(70)	5940(30)	60(10)
H(16A)	4249	-942	7865	35
H(16B)	4457	-769	6779	35
H(17A)	3954	-123	5333	32
H(17B)	3841	-2090	6181	32
H(24A)	3136	-2574	5259	44
H(24B)	3379	-1355	4458	44
H(24C)	2972	-669	4259	44
H(25A)	2794	6852	6901	47
H(25B)	2861	5602	8208	47
H(25C)	2584	4543	7072	47

H(26A)	3418	7697	8110	44
H(26B)	3803	6601	8555	44
H(26C)	3492	5874	9213	44
H(27A)	4119	3887	5698	30
H(27B)	4424	5434	6503	30
H(28A)	4677	4397	8649	56
H(28B)	4869	2327	8103	56
H(28C)	4642	1803	9109	56

Table 6. Torsion angles [°] for CCDC 2115175.

C(9)-O(1)-C(1)-C(13)	163.8(2)
C(9)-O(1)-C(1)-C(14)	-77.6(2)
C(9)-O(1)-C(1)-C(2)	46.0(2)
O(1)-C(1)-C(2)-C(3)	-61.9(3)
C(13)-C(1)-C(2)-C(3)	-175.38(19)
C(14)-C(1)-C(2)-C(3)	60.0(3)
C(1)-C(2)-C(3)-C(4)	45.3(3)
C(2)-C(3)-C(4)-C(9)	-13.7(3)
C(2)-C(3)-C(4)-C(5)	166.1(2)
C(9)-C(4)-C(5)-C(6)	3.4(3)
C(3)-C(4)-C(5)-C(6)	-176.36(19)
C(9)-C(4)-C(5)-C(10)	-176.08(19)
C(3)-C(4)-C(5)-C(10)	4.1(3)
C(4)-C(5)-C(6)-O(2)	-178.7(2)
C(10)-C(5)-C(6)-O(2)	0.8(3)
C(4)-C(5)-C(6)-C(7)	-0.1(3)
C(10)-C(5)-C(6)-C(7)	179.4(2)
O(2)-C(6)-C(7)-C(8)	175.55(19)
C(5)-C(6)-C(7)-C(8)	-3.1(3)
O(2)-C(6)-C(7)-C(11)	-4.7(3)
C(5)-C(6)-C(7)-C(11)	176.7(2)
C(6)-C(7)-C(8)-C(9)	2.9(3)
C(11)-C(7)-C(8)-C(9)	-176.87(19)
C(6)-C(7)-C(8)-C(12)	-178.92(19)
C(11)-C(7)-C(8)-C(12)	1.3(3)
C(1)-O(1)-C(9)-C(4)	-14.4(3)
C(1)-O(1)-C(9)-C(8)	166.46(18)
C(5)-C(4)-C(9)-O(1)	177.28(18)
C(3)-C(4)-C(9)-O(1)	-2.9(3)
C(5)-C(4)-C(9)-C(8)	-3.6(3)
C(3)-C(4)-C(9)-C(8)	176.15(19)
C(7)-C(8)-C(9)-O(1)	179.57(18)
C(12)-C(8)-C(9)-O(1)	1.4(3)
C(7)-C(8)-C(9)-C(4)	0.4(3)
C(12)-C(8)-C(9)-C(4)	-177.75(19)
O(1)-C(1)-C(13)-O(3)	62.3(3)

C(14)-C(1)-C(13)-O(3)	-55.6(3)
C(2)-C(1)-C(13)-O(3)	178.8(2)
C(23)-O(4)-C(15)-C(16)	-46.6(2)
C(23)-O(4)-C(15)-C(28)	-167.0(2)
C(23)-O(4)-C(15)-C(27)	75.4(2)
O(4)-C(15)-C(16)-C(17)	59.3(2)
C(28)-C(15)-C(16)-C(17)	175.19(17)
C(27)-C(15)-C(16)-C(17)	-59.0(2)
C(15)-C(16)-C(17)-C(18)	-42.2(3)
C(16)-C(17)-C(18)-C(23)	13.2(3)
C(16)-C(17)-C(18)-C(19)	-167.45(19)
C(23)-C(18)-C(19)-C(20)	-3.0(3)
C(17)-C(18)-C(19)-C(20)	177.67(18)
C(23)-C(18)-C(19)-C(24)	176.24(19)
C(17)-C(18)-C(19)-C(24)	-3.1(3)
C(18)-C(19)-C(20)-O(5)	179.24(19)
C(24)-C(19)-C(20)-O(5)	0.0(3)
C(18)-C(19)-C(20)-C(21)	0.6(3)
C(24)-C(19)-C(20)-C(21)	-178.6(2)
O(5)-C(20)-C(21)-C(22)	-176.09(19)
C(19)-C(20)-C(21)-C(22)	2.6(3)
O(5)-C(20)-C(21)-C(25)	4.1(3)
C(19)-C(20)-C(21)-C(25)	-177.2(2)
C(20)-C(21)-C(22)-C(23)	-3.3(3)
C(25)-C(21)-C(22)-C(23)	176.50(19)
C(20)-C(21)-C(22)-C(26)	177.76(19)
C(25)-C(21)-C(22)-C(26)	-2.4(3)
C(15)-O(4)-C(23)-C(18)	17.5(3)
C(15)-O(4)-C(23)-C(22)	-164.04(18)
C(19)-C(18)-C(23)-O(4)	-179.39(19)
C(17)-C(18)-C(23)-O(4)	0.0(3)
C(19)-C(18)-C(23)-C(22)	2.3(3)
C(17)-C(18)-C(23)-C(22)	-178.39(19)
C(21)-C(22)-C(23)-O(4)	-177.51(18)
C(26)-C(22)-C(23)-O(4)	1.4(3)
C(21)-C(22)-C(23)-C(18)	0.9(3)
C(26)-C(22)-C(23)-C(18)	179.84(19)
O(4)-C(15)-C(27)-O(6)	-173.90(16)

C(16)-C(15)-C(27)-O(6)	-53.4(2)
C(28)-C(15)-C(27)-O(6)	72.8(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for CCDC 2115175 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(6)-H(6)...O(3)	0.84(3)	1.90(3)	2.725(2)	167(4)
O(5)-H(5)...O(5)#1	0.88(3)	2.47(3)	3.2899(15)	156(3)
O(3)-H(3)...O(6)#2	0.82(3)	2.05(3)	2.783(2)	149(3)
O(2)-H(2)...O(2)#3	0.87(3)	2.50(3)	3.3356(15)	163(3)

Symmetry transformations used to generate equivalent atoms:

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