Supporting information

Synthesis of chiral cyclohexanol derived benzylamines, applications for enantiodiscrimination of optically active analytes by NMR spectroscopy

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1. Characterization data:

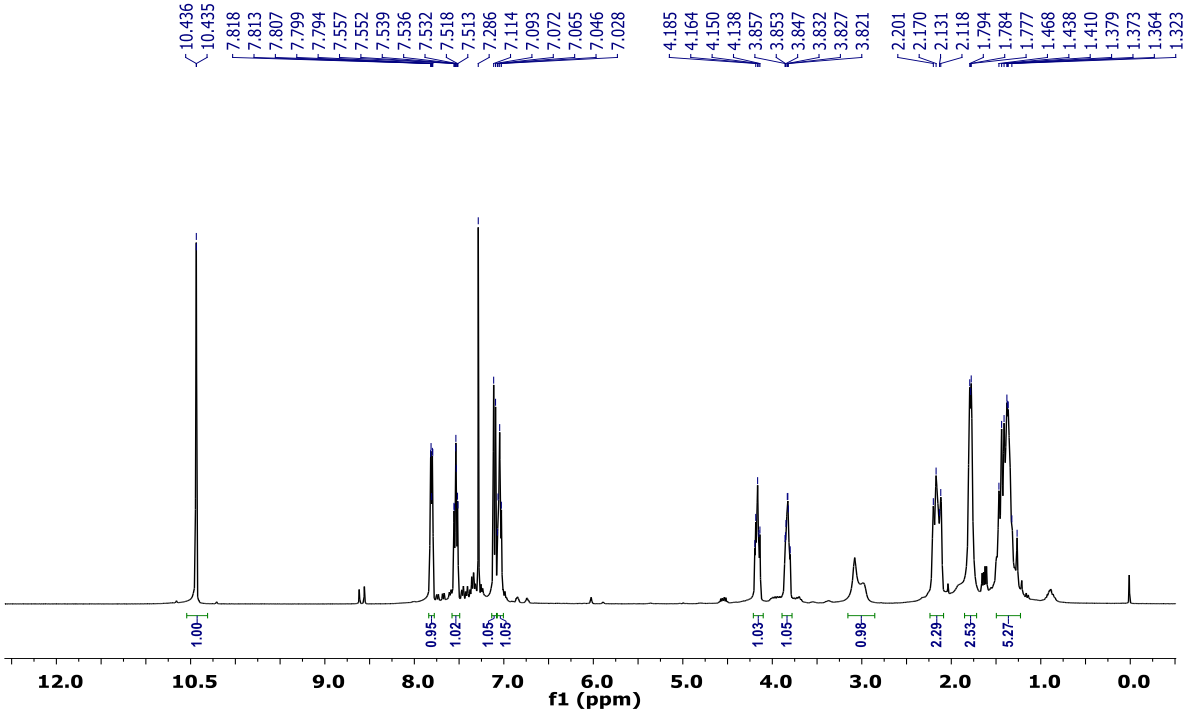


Figure 1: ^{1}H NMR of **1**

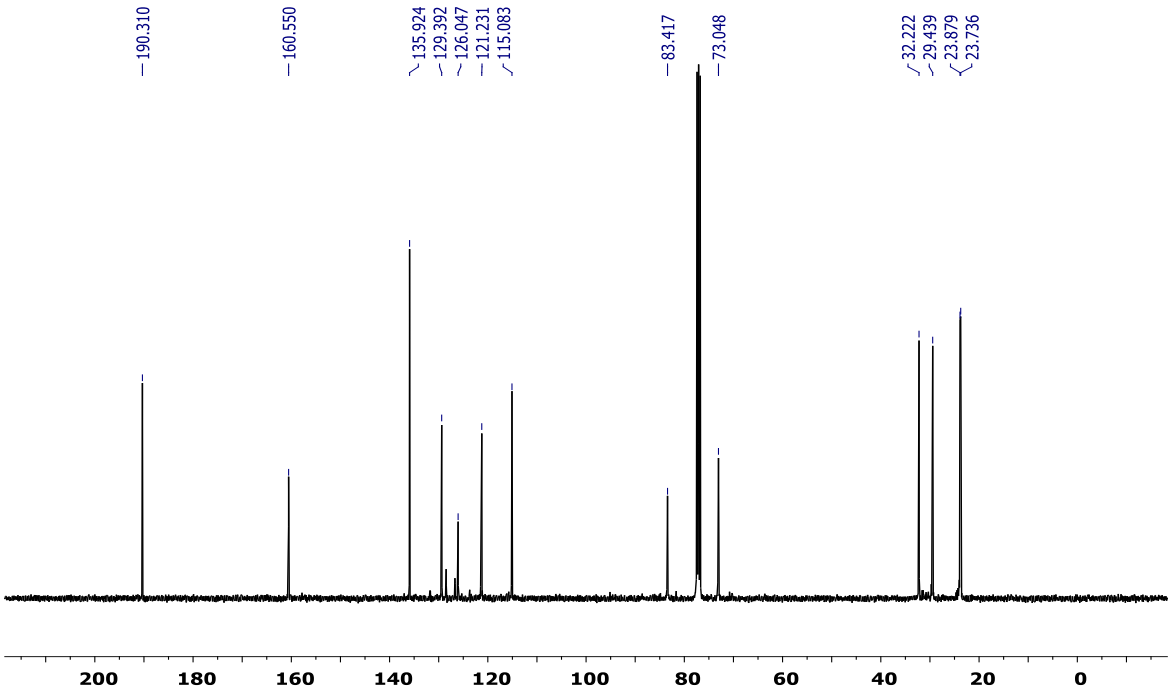
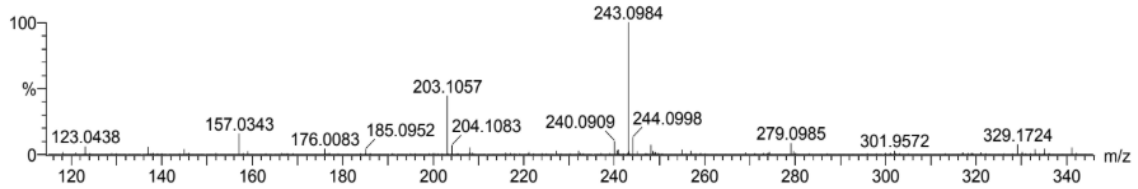


Figure 2: ^{13}C NMR of **1**

Monoisotopic Mass, Even Electron Ions
47 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-14 H: 0-40 N: 0-3 O: 0-4 Na: 1-1

040123_BP_08 27 (0.294) IITRPR XEVO G2-XS QTOF
Test Name : 040123_BP_08
1: TOF MS ES+
2.61e+006



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
243.0984	243.0997	-1.3	-5.3	5.5	1125.4	n/a	n/a	C13 H16 O3 Na

Figure 3: HRMS of **1**

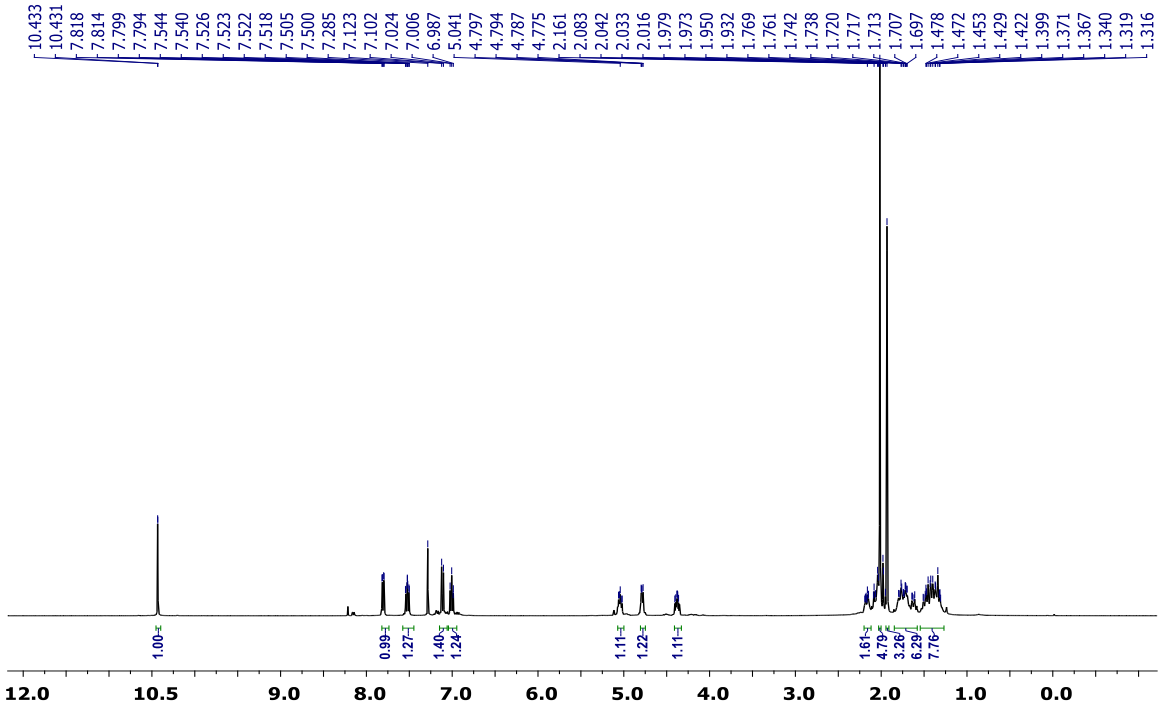


Figure 4: ^{1}H NMR of **2**

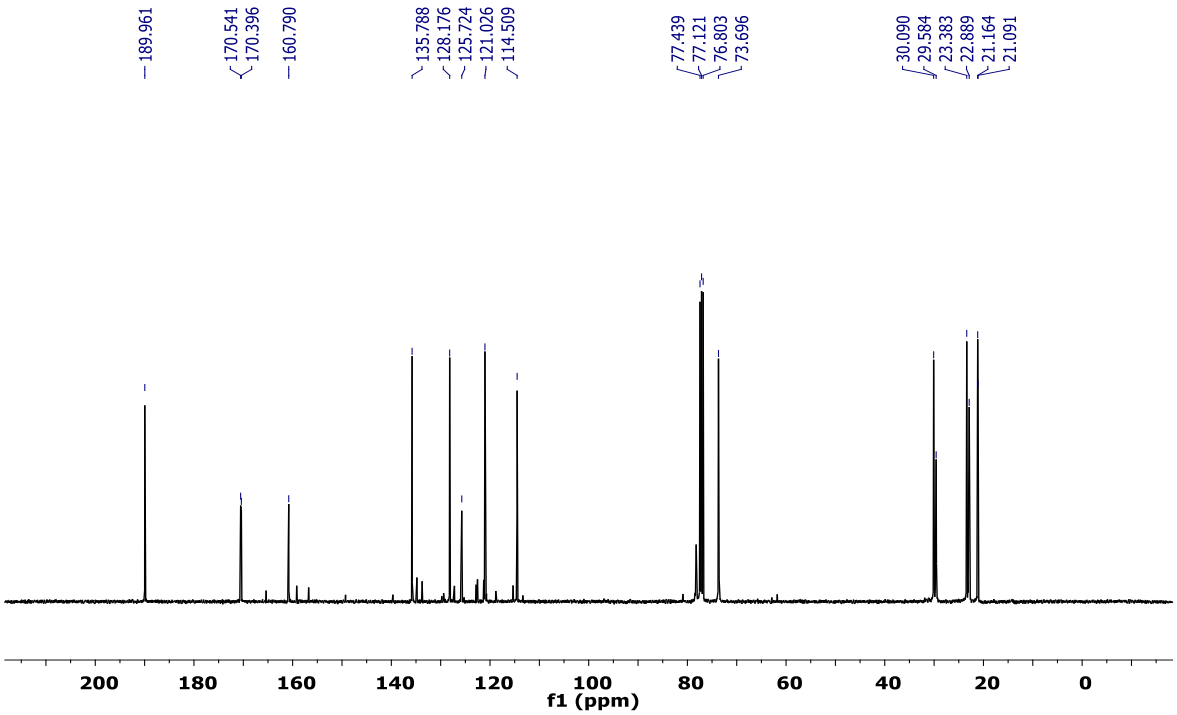


Figure 5: ^{13}C NMR of **2**

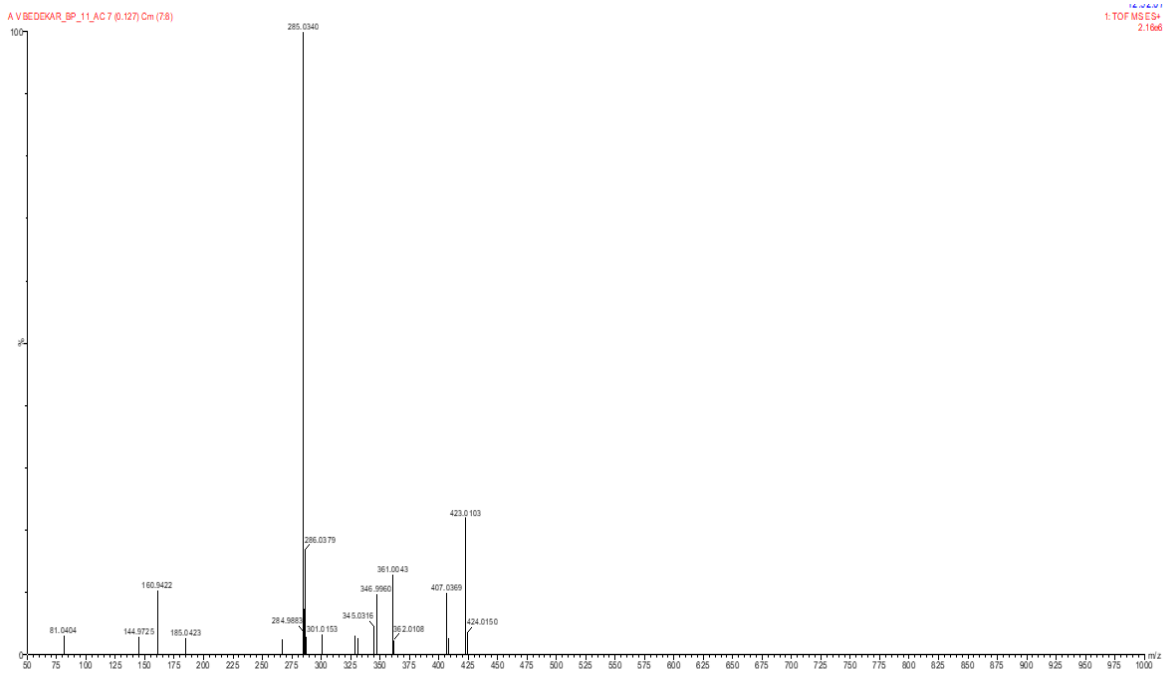
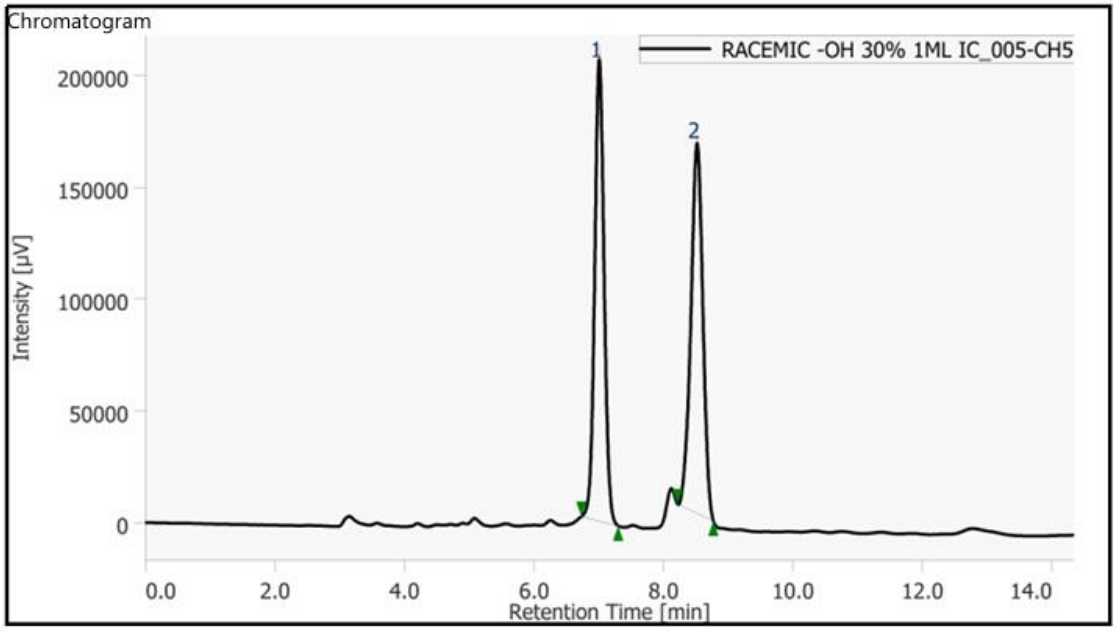


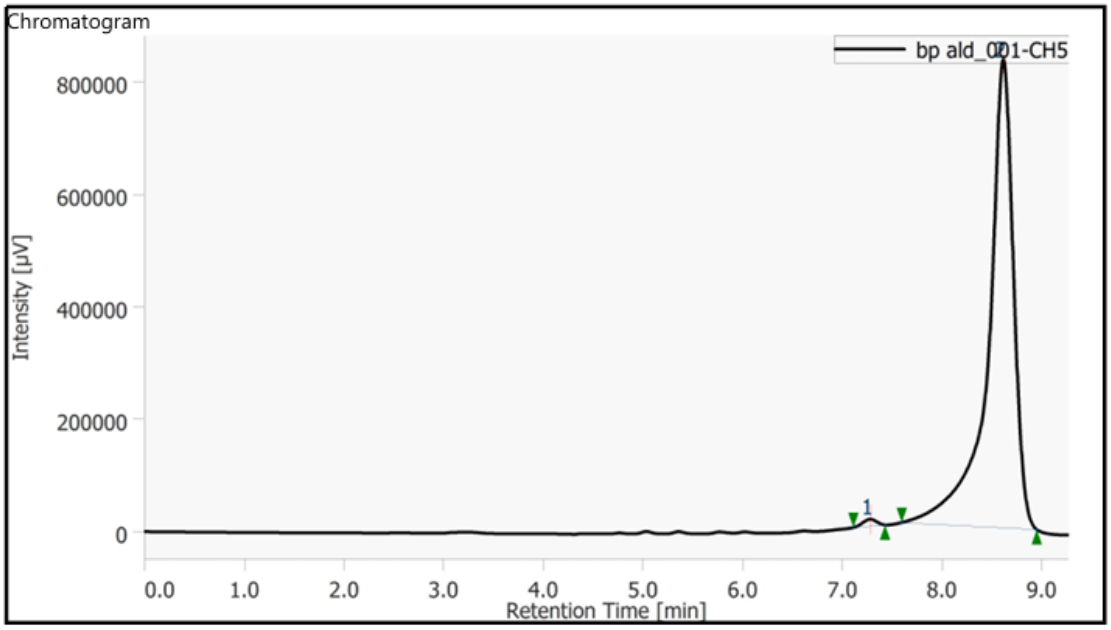
Figure 6: HRMS of **2**



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	5	7.003	2078161	206328	49.528	55.499	N/A	11485	5.065	1.033	
2	Unknown	5	8.510	2117806	165438	50.472	44.501	N/A	10314	N/A	0.951	

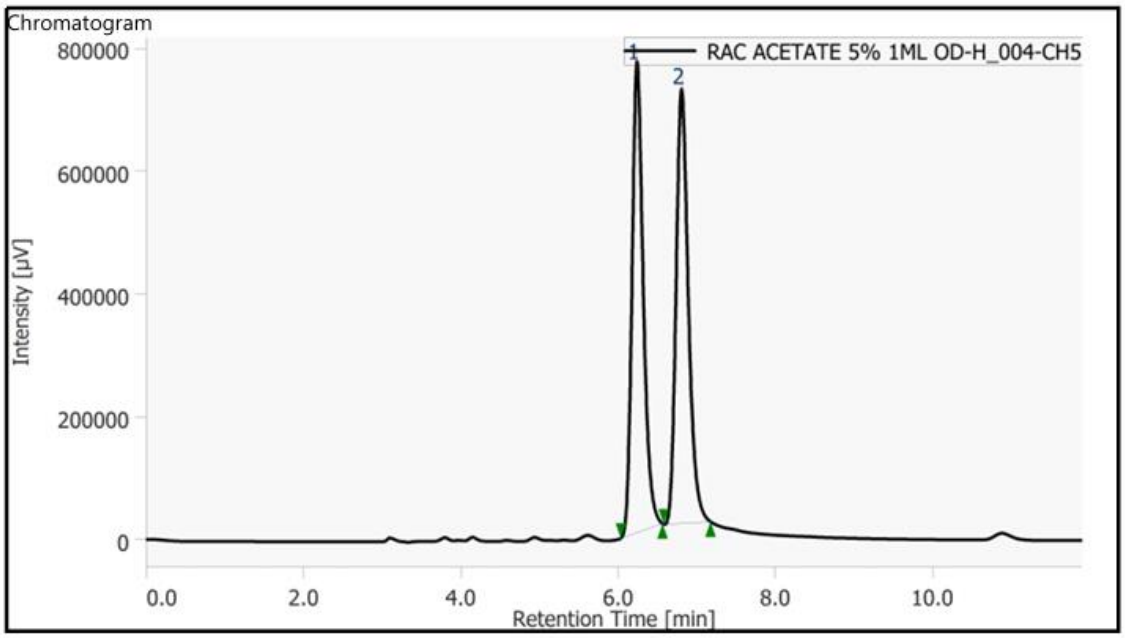
Figure 7: HPLC of Racemic **1**



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	5	7.277	117869	12254	0.795	1.451	N/A	11956	4.129	0.925	
2	Unknown	5	8.610	14701299	832327	99.205	98.549	N/A	8158	N/A	0.698	

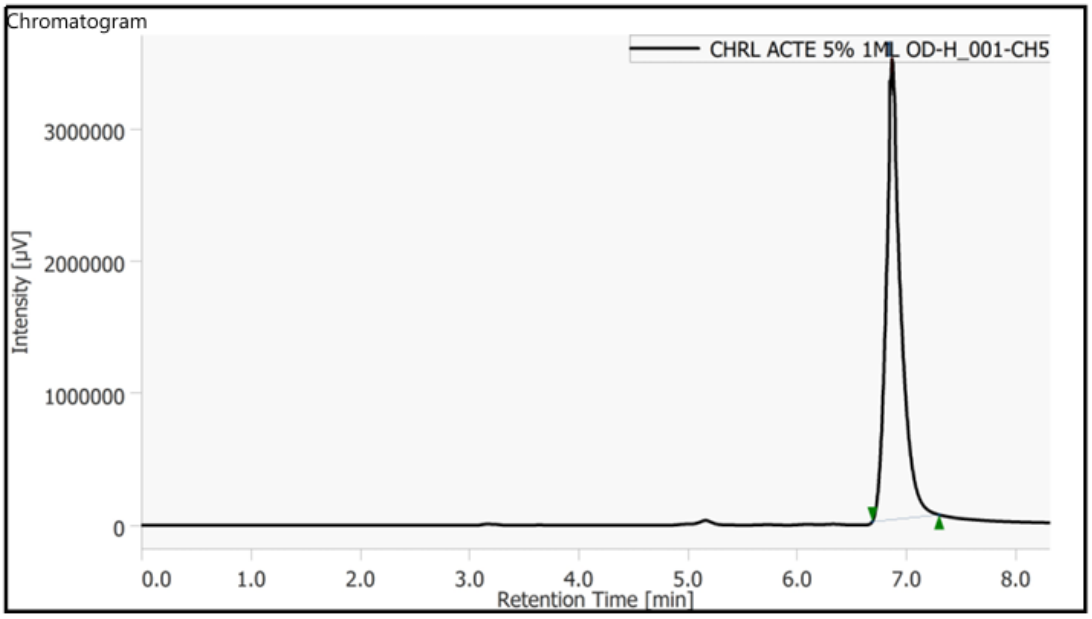
Figure 8: HPLC of Chiral alcohol (*S*,*S*)-**1**



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	5	6.237	7630584	767283	49.955	52.042	N/A	9631	2.138	1.278	
2	Unknown	5	6.803	7644369	707057	50.045	47.958	N/A	9637	N/A	1.280	

Figure 9: HPLC of Racemic acetate **2**



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	5	6.863	32166808	3485339	100.000	100.000	N/A	16014	N/A	1.371	

Figure 10: HPLC of Chiral acetate (*R*,*R*)-**2**

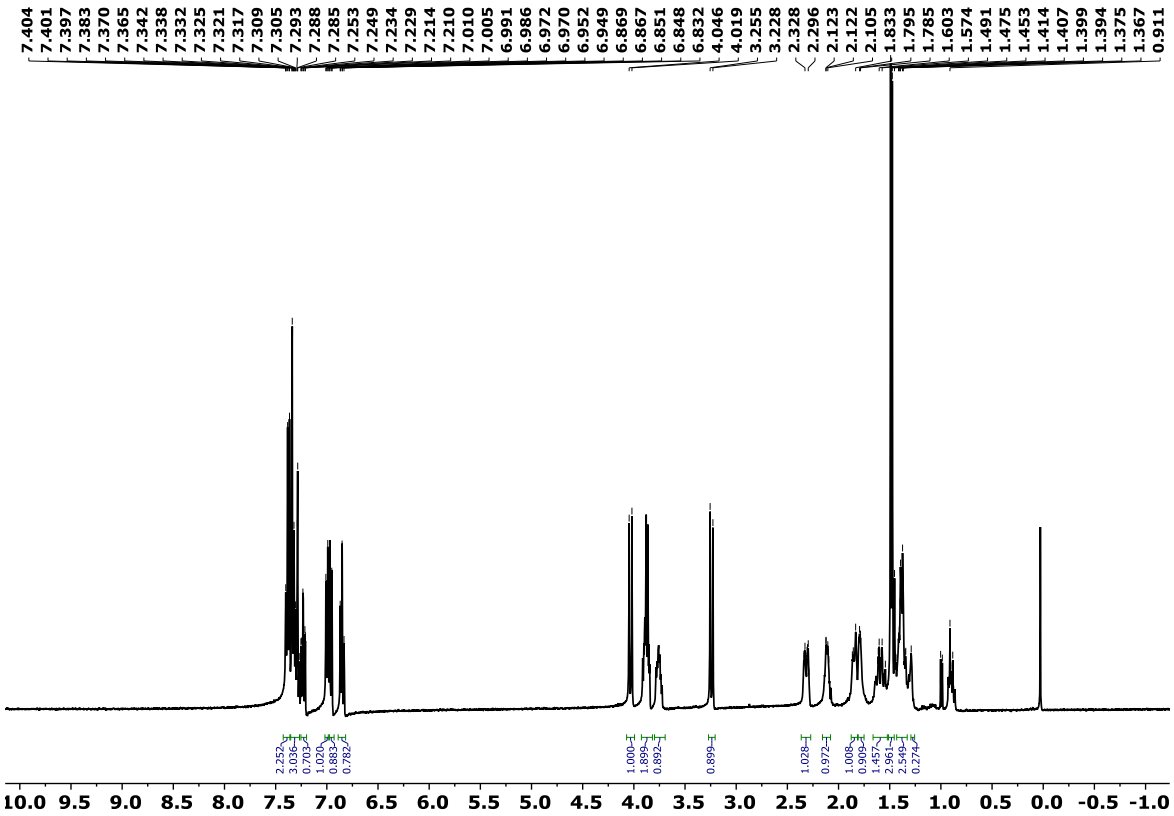


Figure 11: ^{1}H NMR of (*R*,*R*,*S*)-**4**

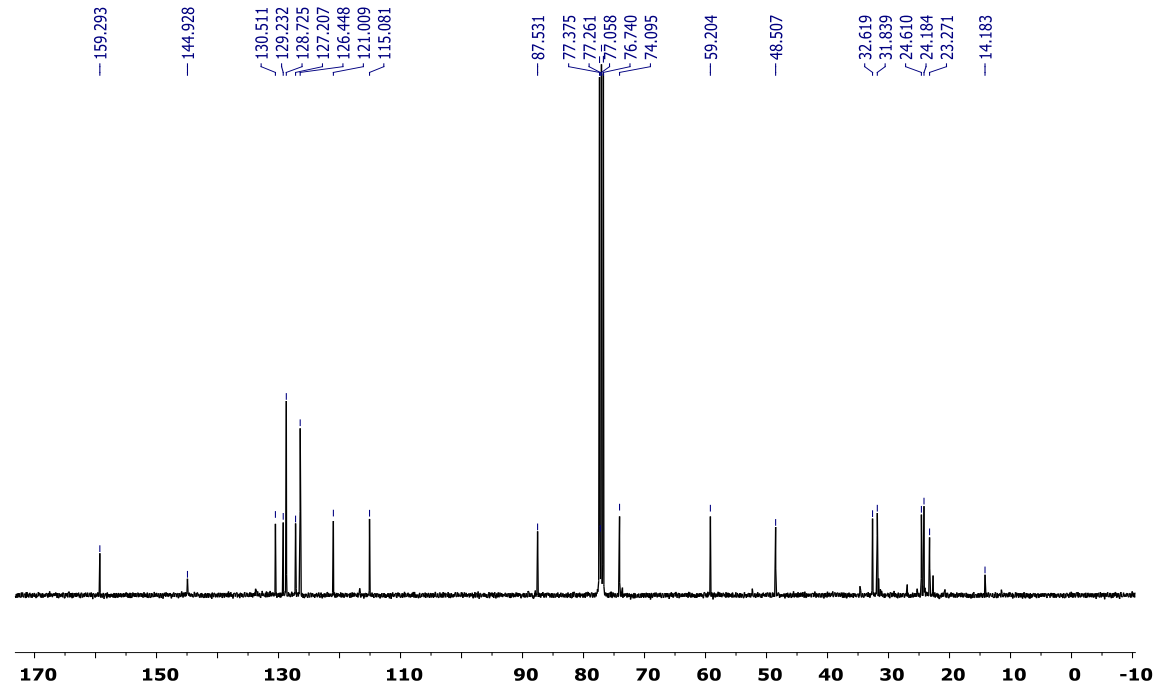


Figure 12: ^{13}C NMR of (*R*,*R*,*S*)-**4**

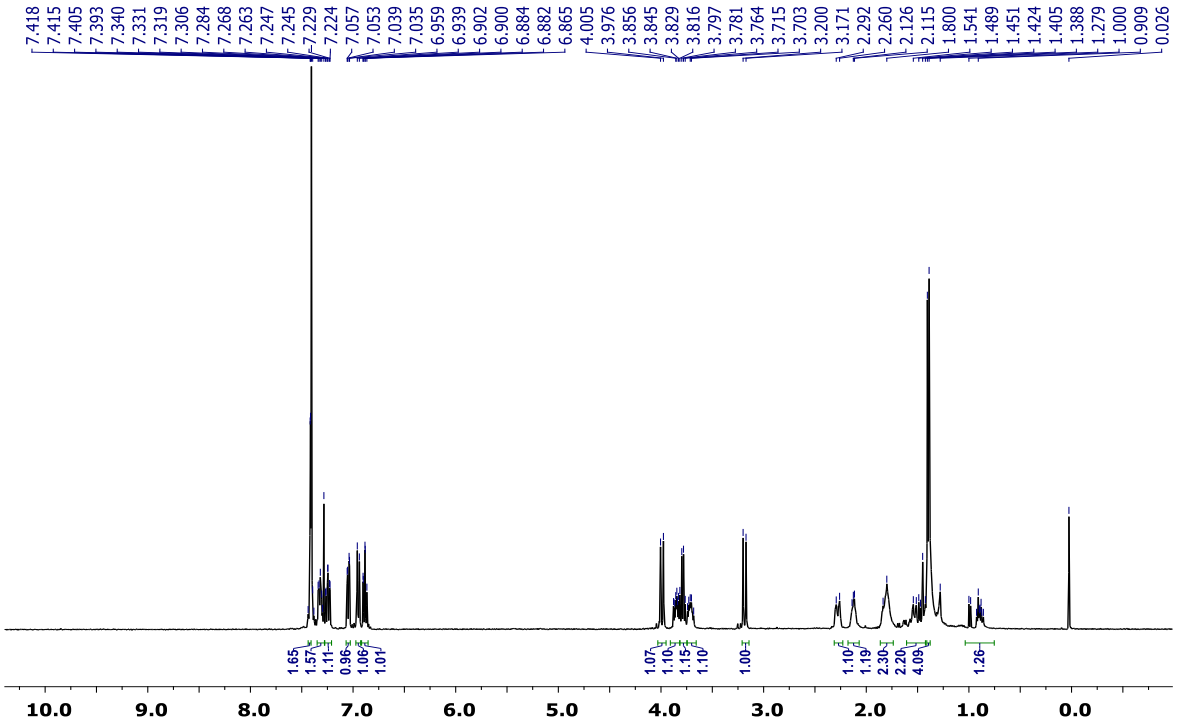
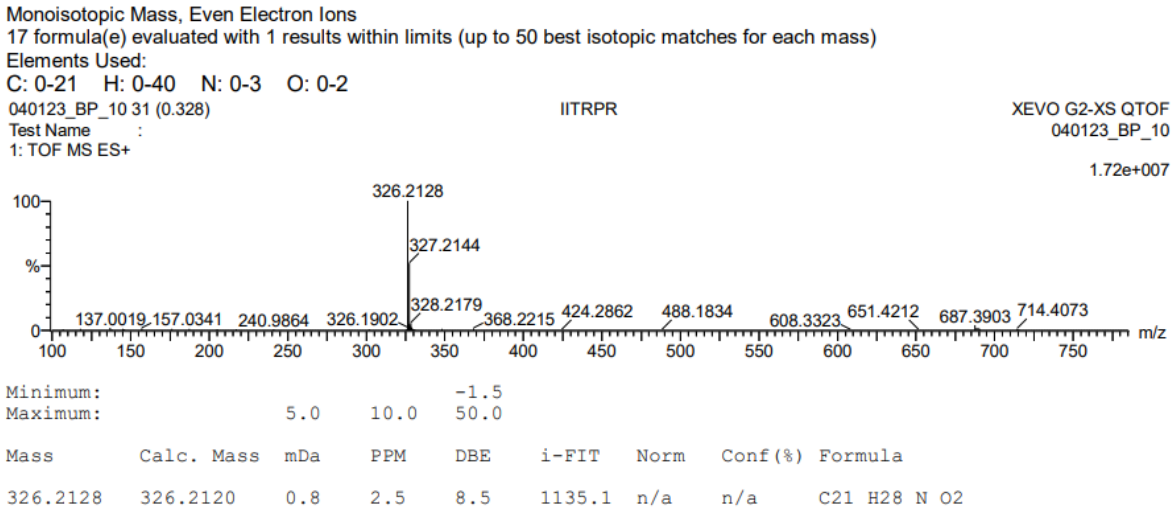


Figure 13: ^{1}H NMR of (*S*,*S*,*S*)-**4**



Monoisotopic Mass, Even Electron Ions
17 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-21 H: 0-40 N: 0-3 O: 0-2

040123_BP_10 31 (0.328) IITRPR XEVO G2-XS QTOF
Test Name : 040123_BP_10
1: TOF MS ES+ 1.72e+007

Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
326.2128	326.2120	0.8	2.5	8.5	1135.1	n/a	n/a	C21 H28 N O2

Figure 14: HRMS of (*S*,*S*,*S*)-**4**

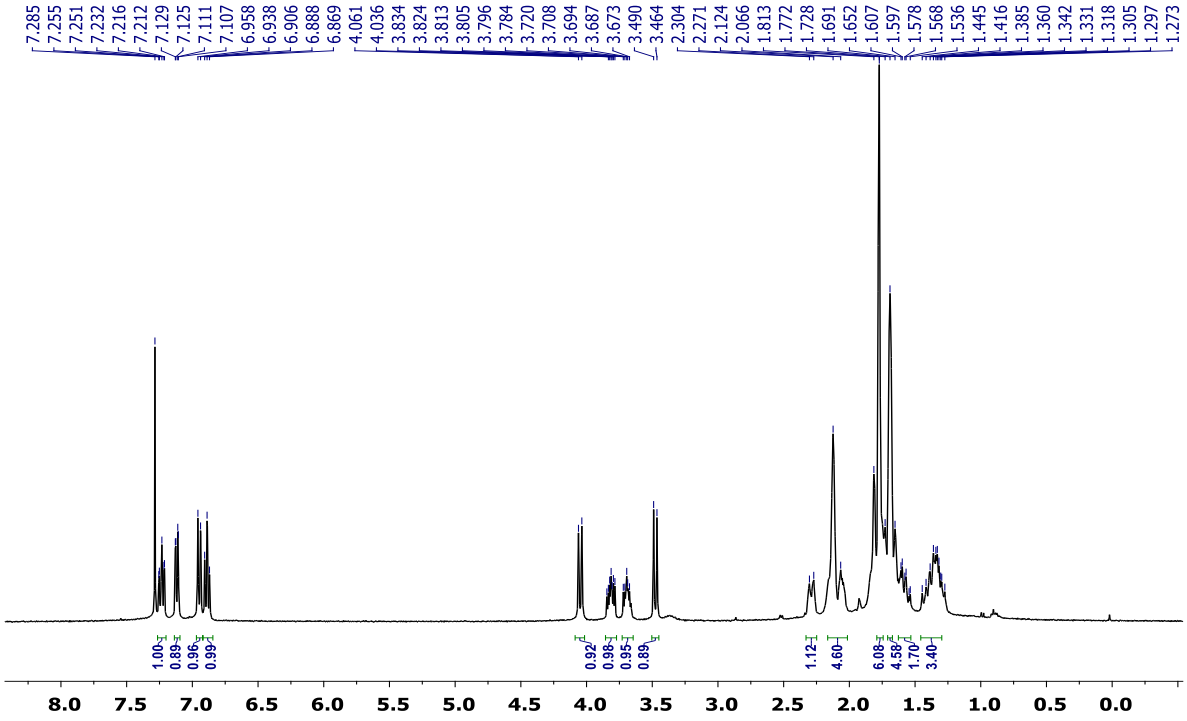


Figure 15: ^{1}H NMR of (*S*,*S*)-**6**

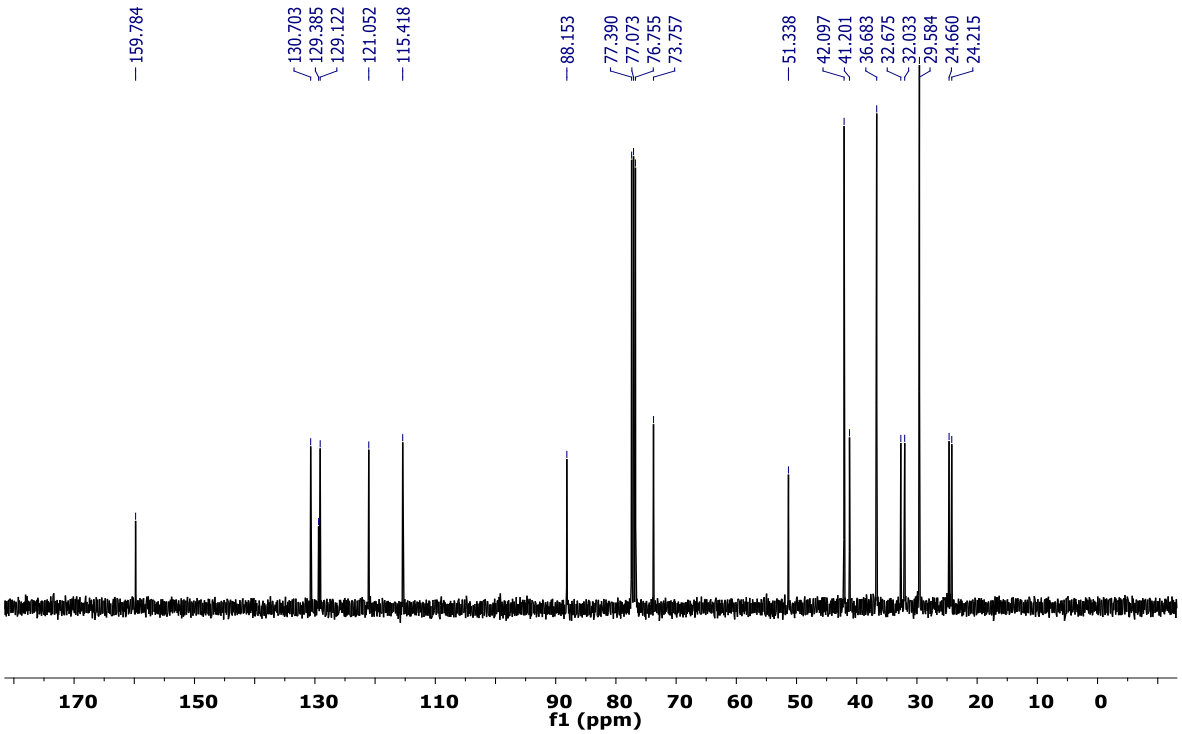


Figure 16: ^{13}C NMR of (*S*,*S*)-**6**

Optimization of concentration of CSA experiments:

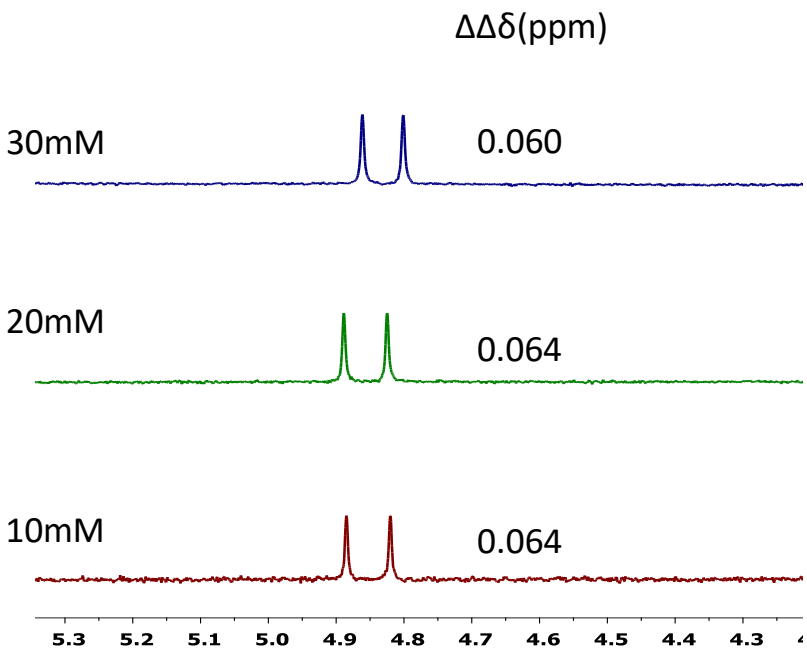


Figure 17: Concentration study

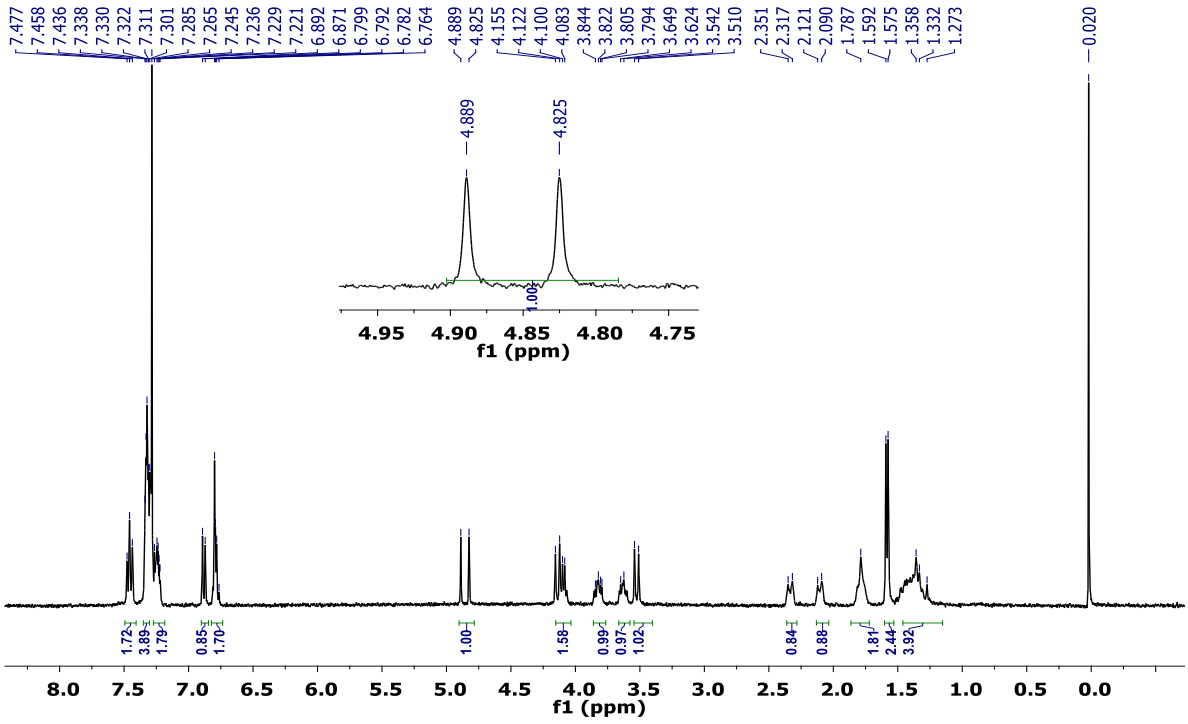


Figure 18: ^{1}H NMR spectra of **7** with (*R*,*R*,*S*)-**4**

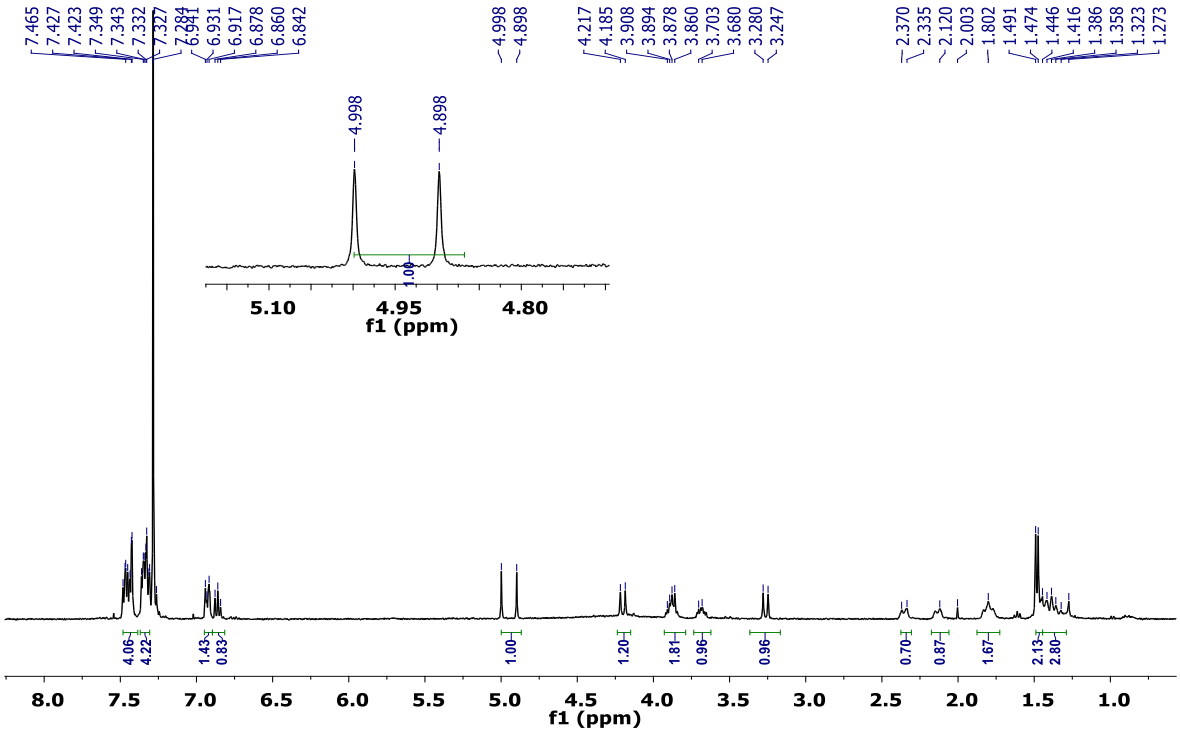


Figure 19: ^{1}H NMR spectra of **7** with (*S*,*S*,*S*)-**4**

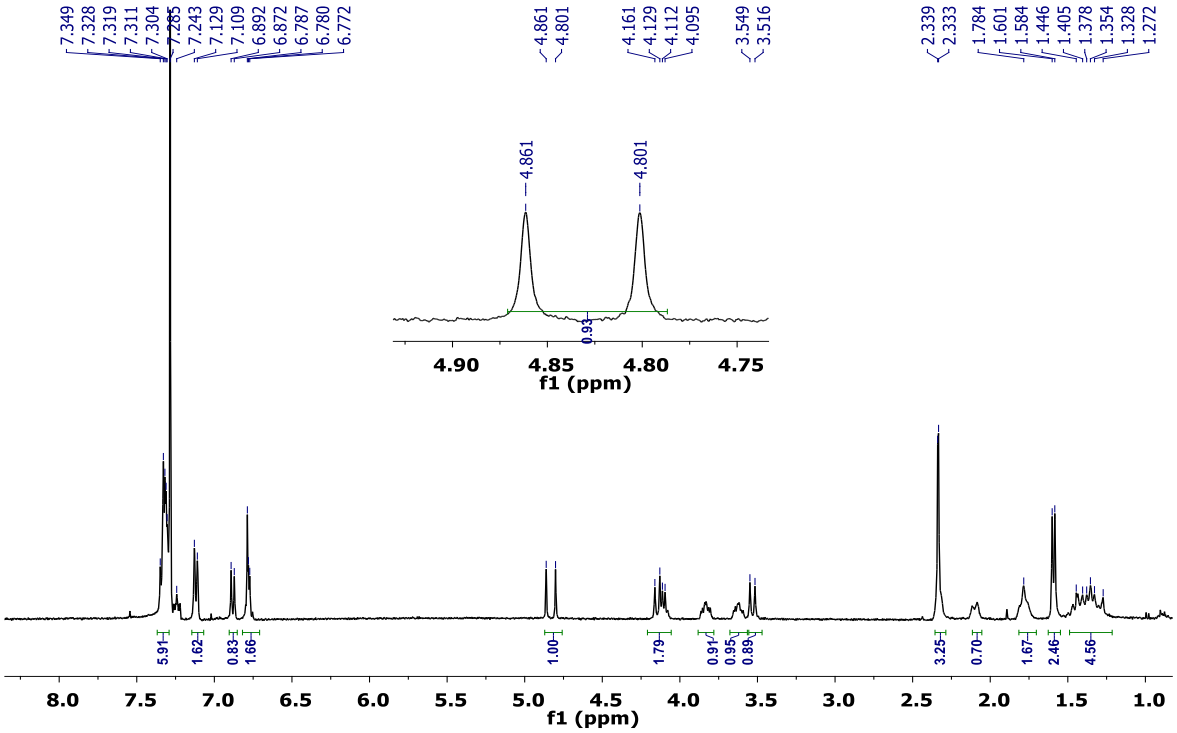


Figure 20: ^{1}H NMR spectra of **8** with (*R*,*R*,*S*)-**4**

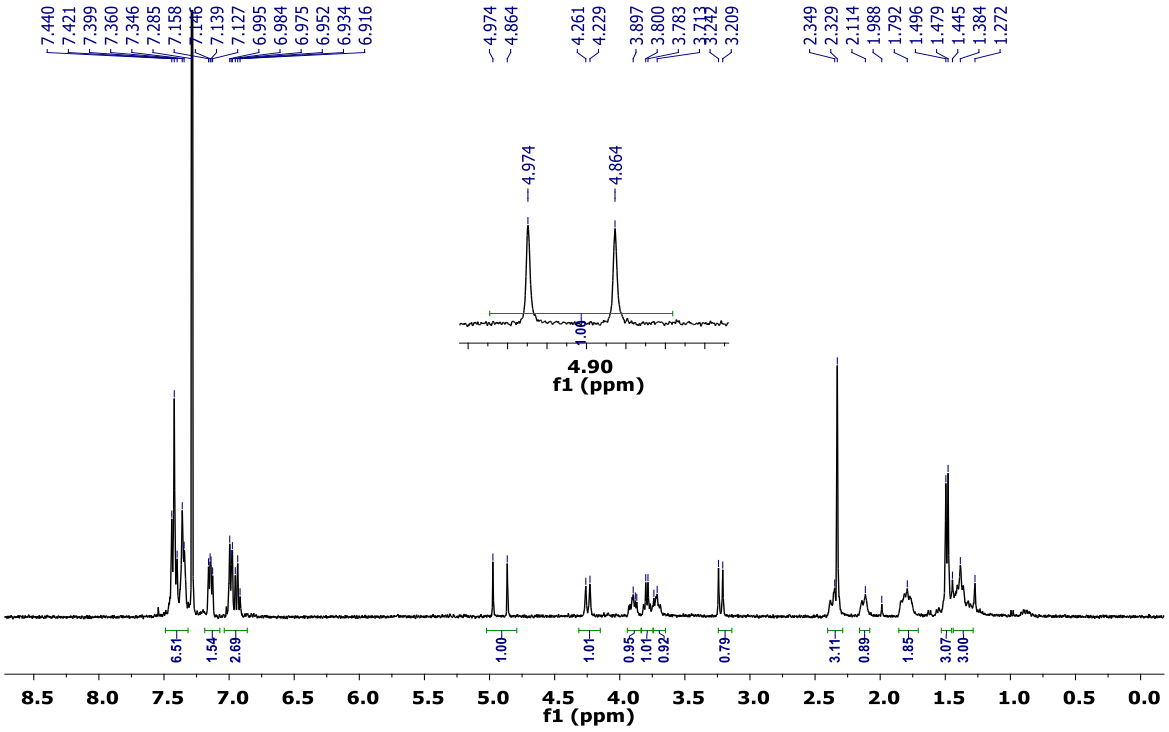


Figure 21: ^{1}H NMR spectra of **8** with (*S*,*S*,*S*)-**4**

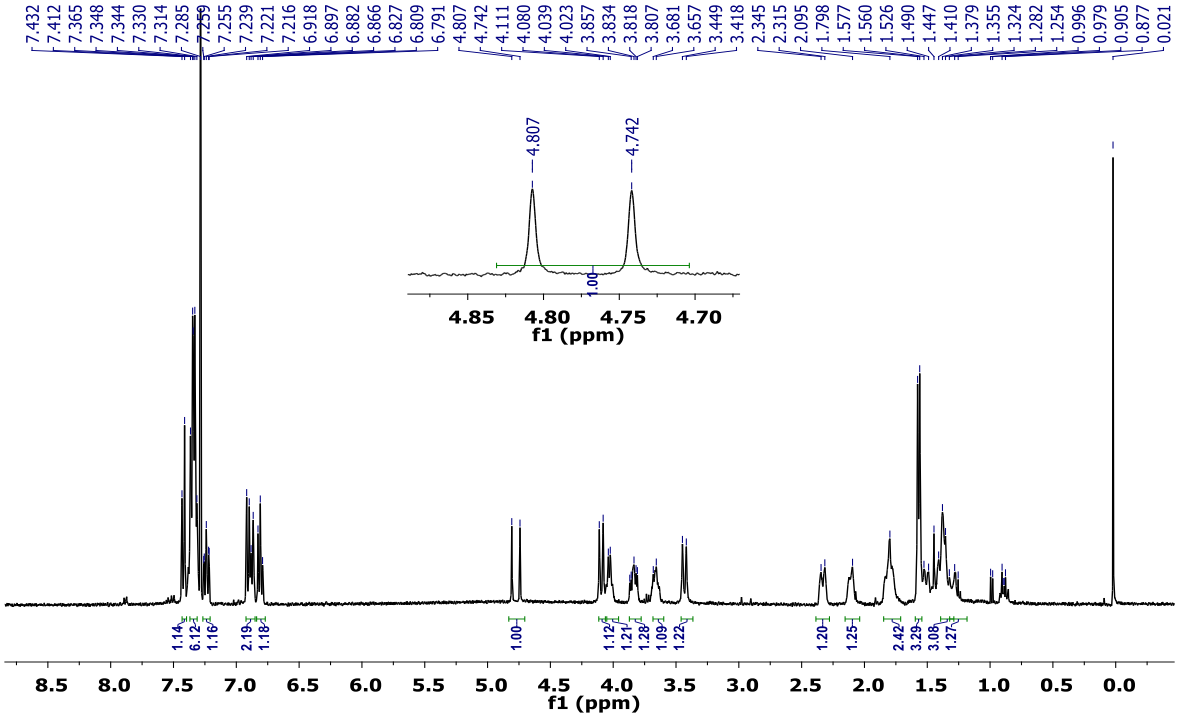


Figure 22: ^{1}H NMR spectra of **9** with (*R*,*R*,*S*)-**4**

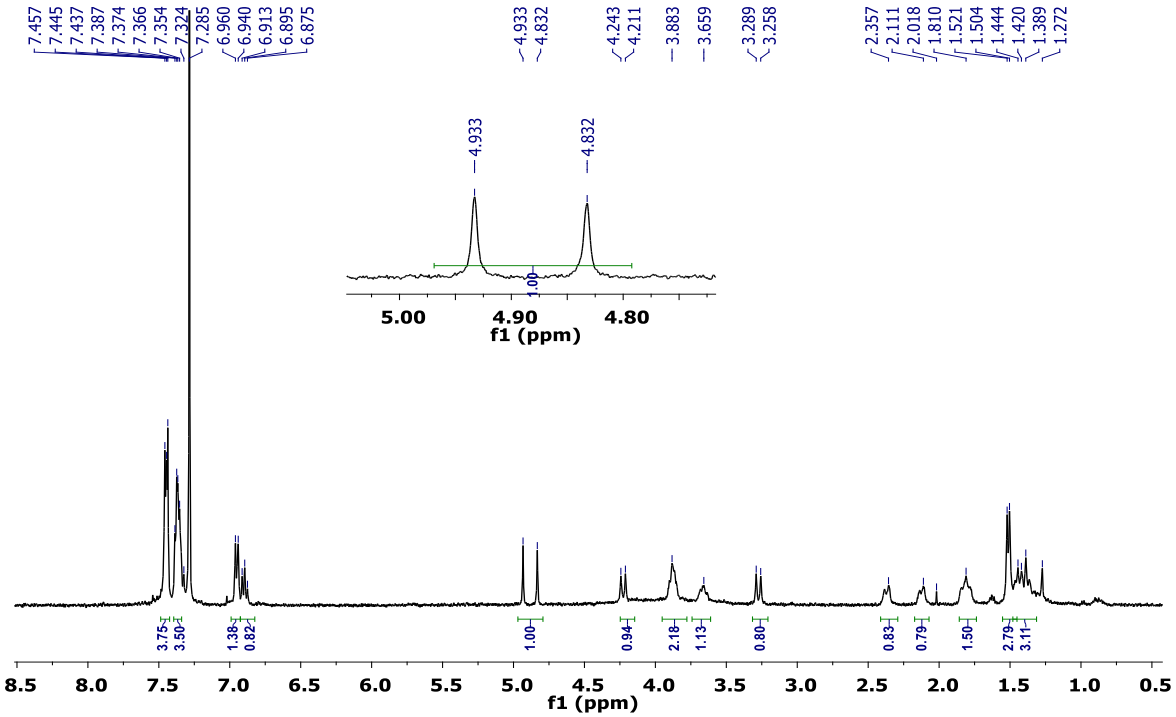


Figure 23: ^{1}H NMR spectra of **9** with (*S*,*S*,*S*)-**4**

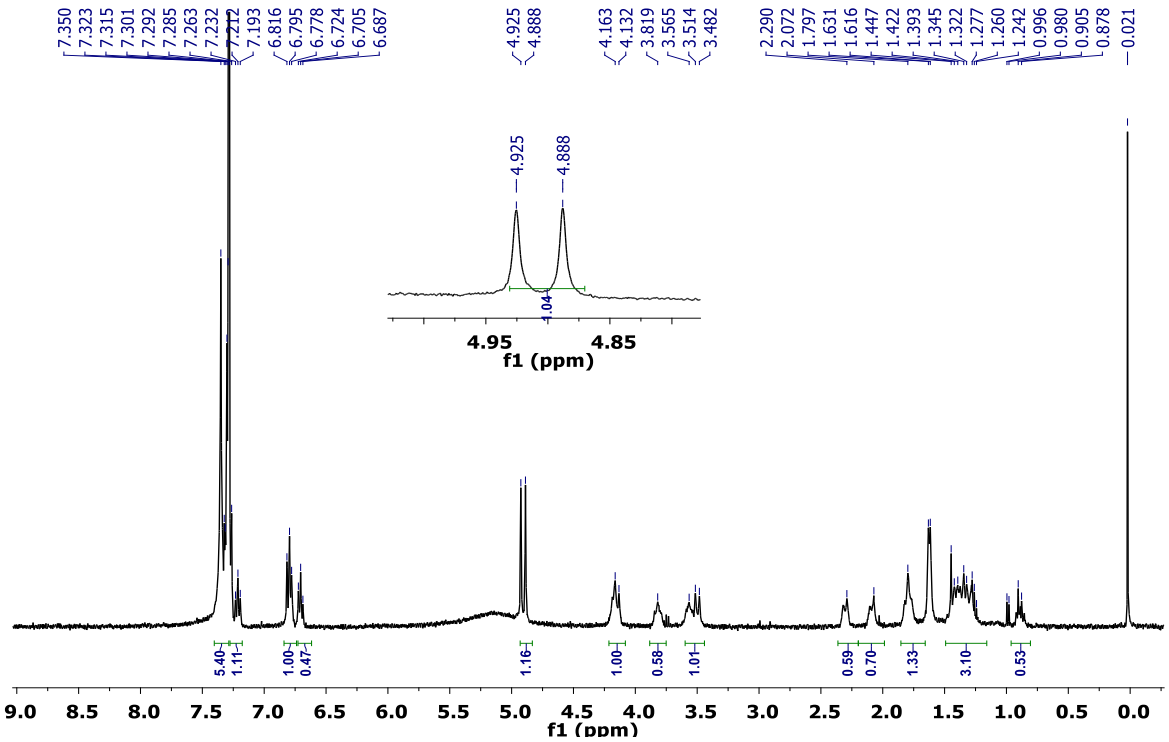


Figure 24: ^{1}H NMR spectra of **10** with (*R*,*R*,*S*)-**4**

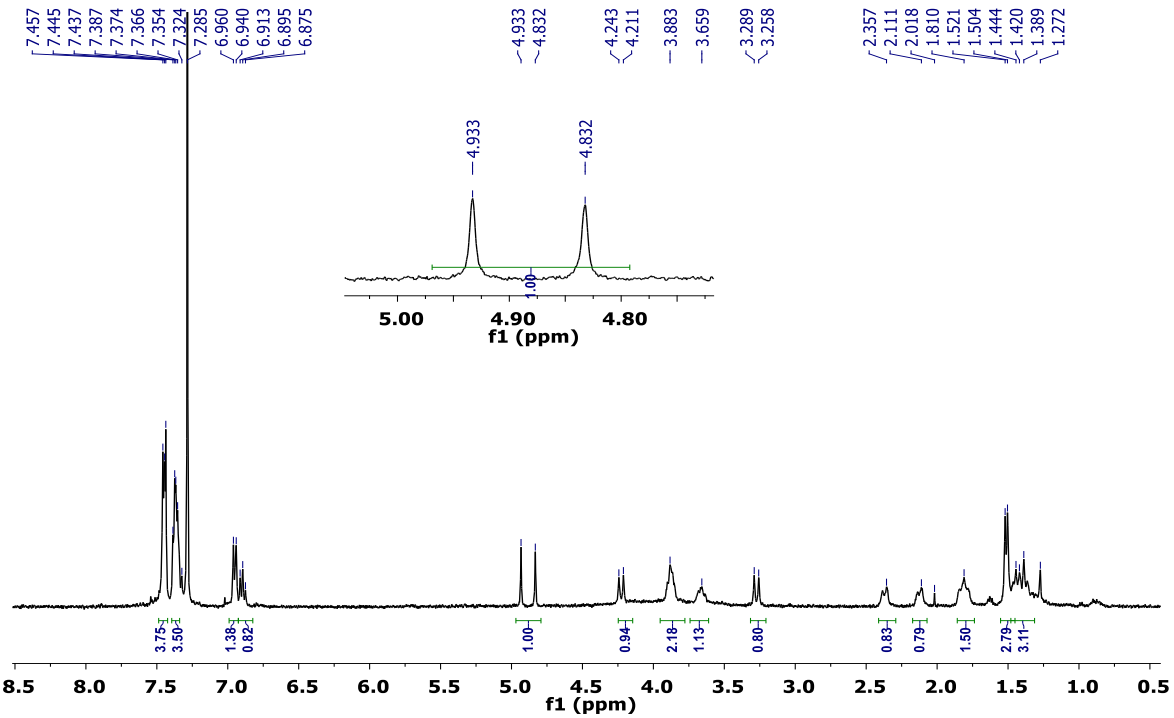


Figure 25: ^{1}H NMR spectra of **10** with (*S*,*S*,*S*)-**4**

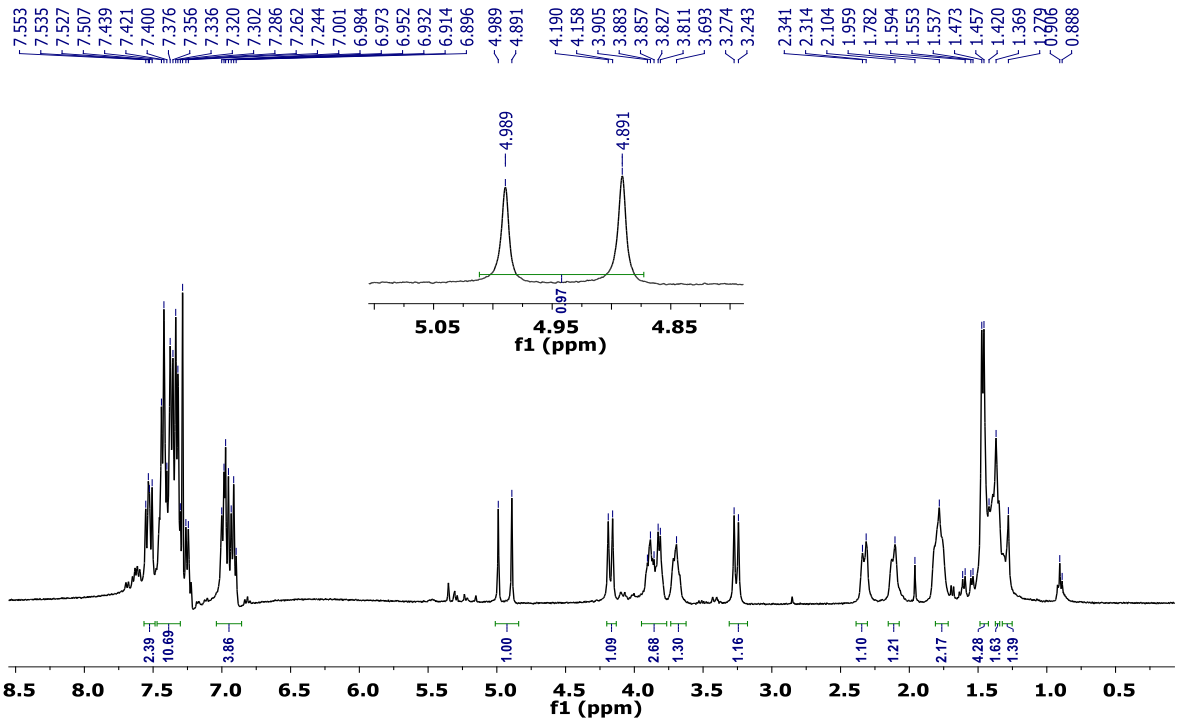


Figure 26: ^{1}H NMR spectra of **11** with (*R*,*R*,*S*)-**4**

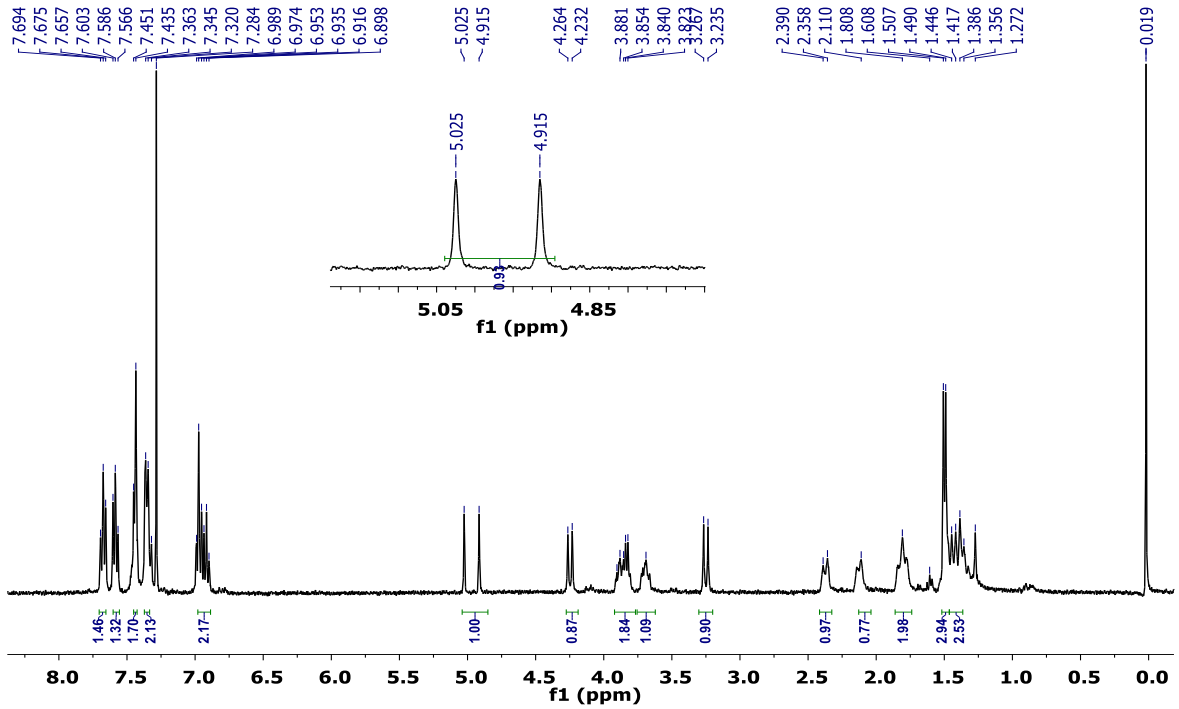


Figure 27: ^{1}H NMR spectra of **11** with (*S*,*S*,*S*)-**4**

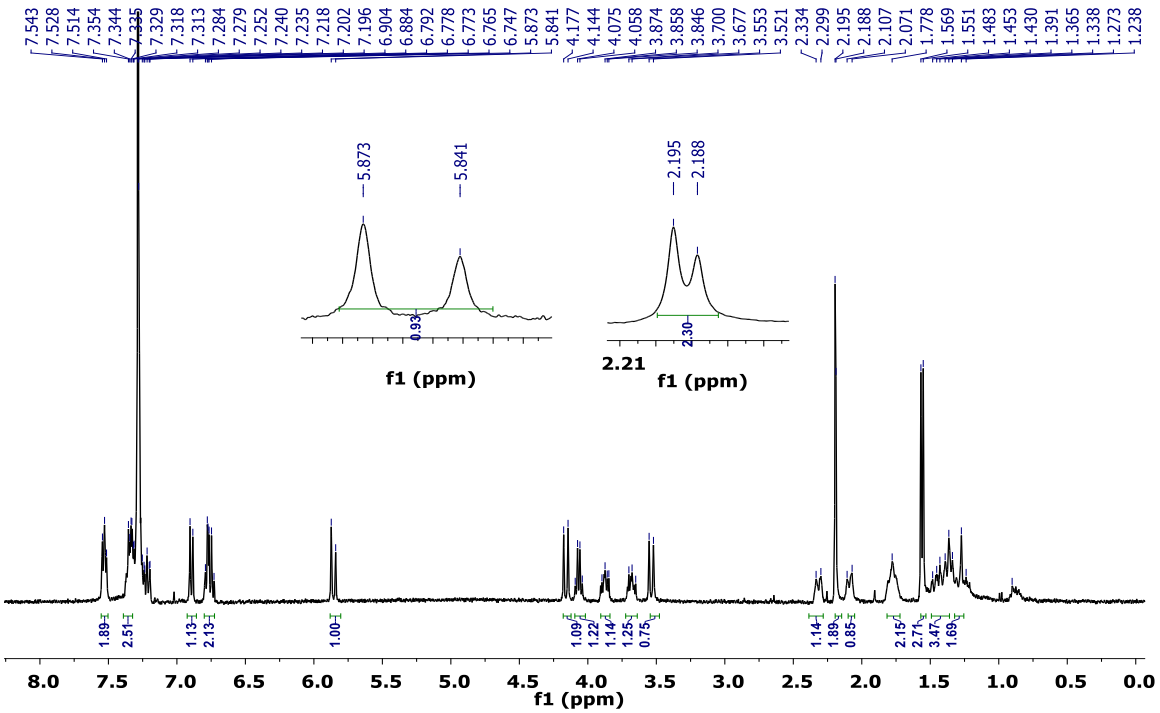


Figure 28: ^{1}H NMR spectra of **12** with (*R*,*R*,*S*)-**4**

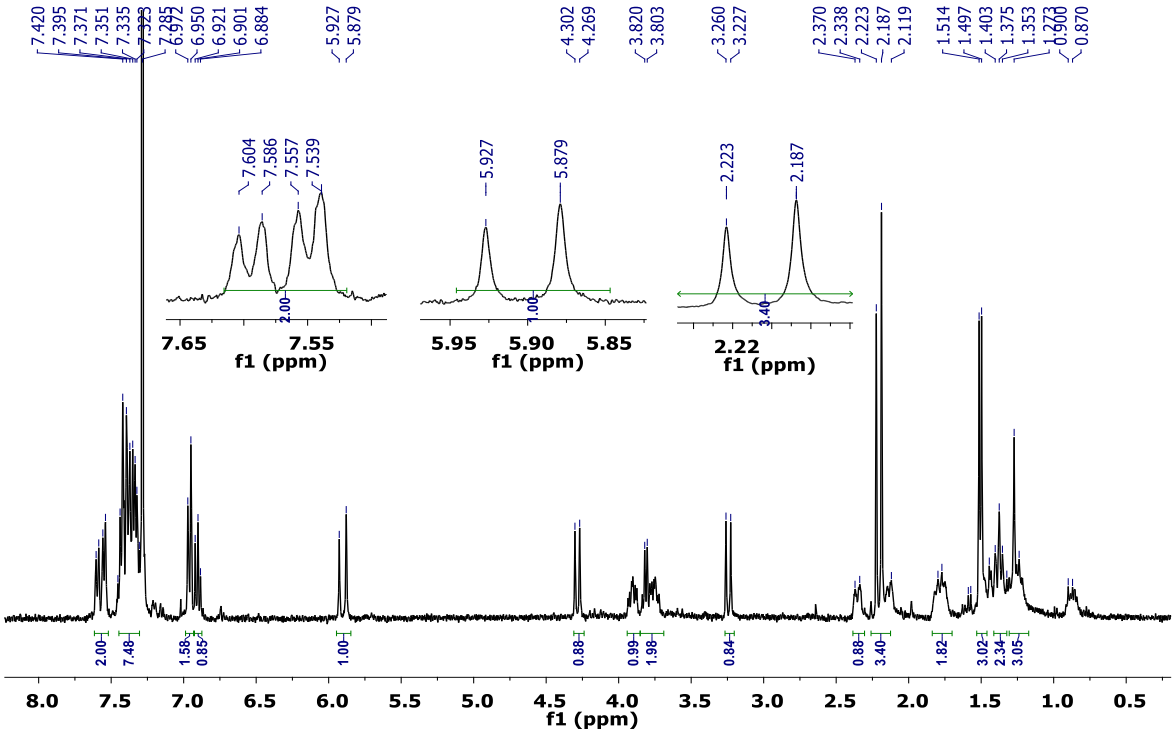


Figure 29: ^{1}H NMR spectra of **12** with (*S*,*S*,*S*)-**4**

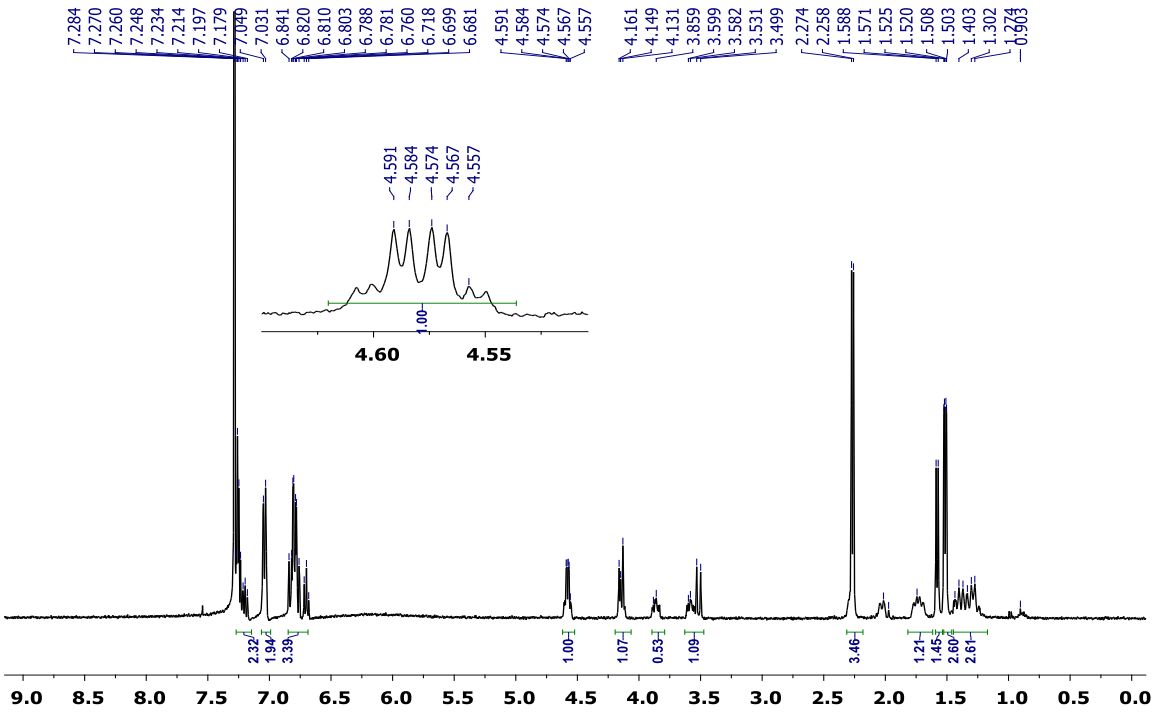


Figure 30: ^{1}H NMR spectra of **14** with (*R*,*R*,*S*)-**4**

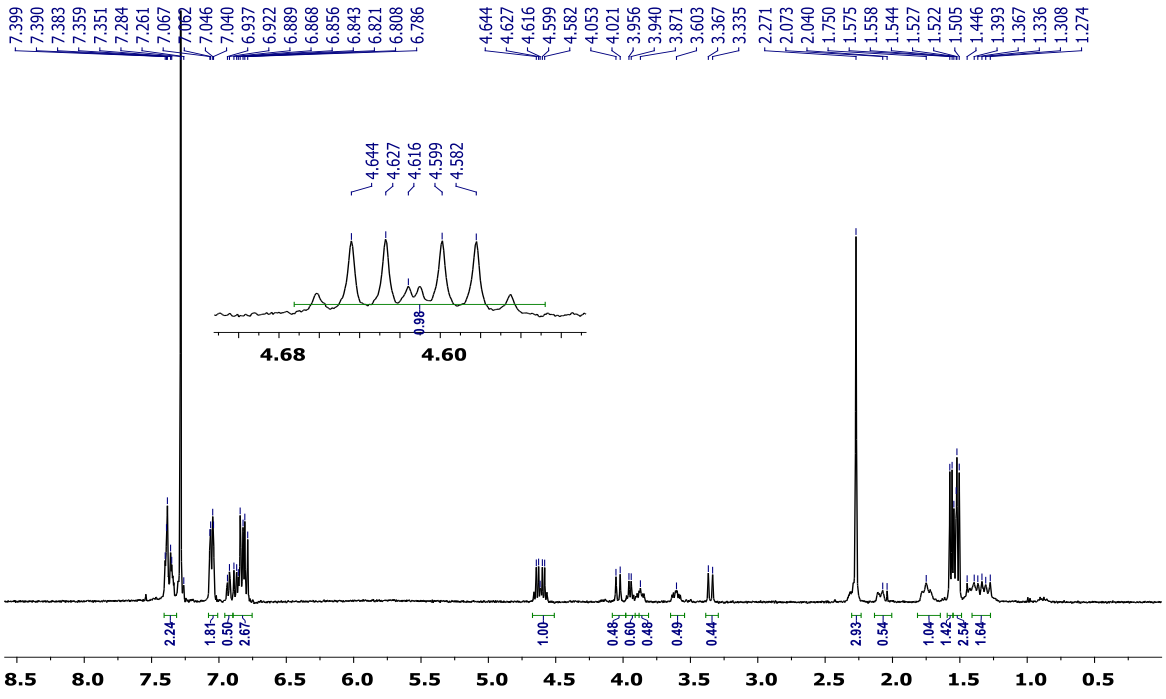


Figure 31: ^{1}H NMR spectra of **14** with (*S*,*S*,*S*)-**4**

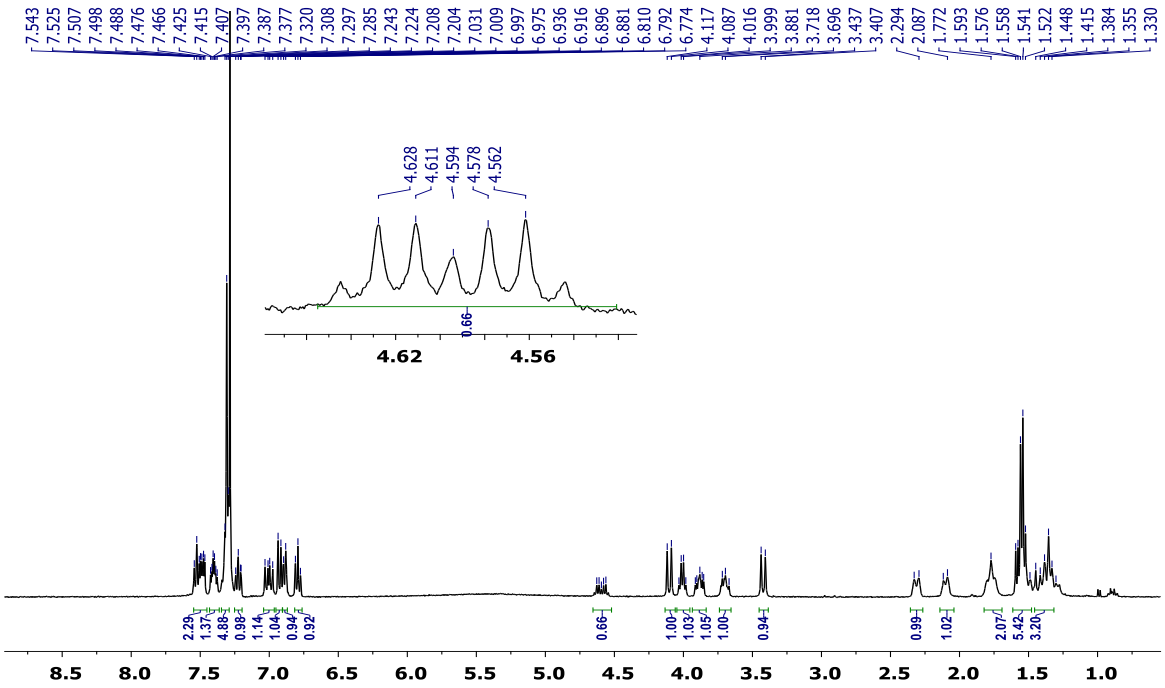


Figure 32: ^{1}H NMR spectra of **15** with (*R*,*R*,*S*)-**4**

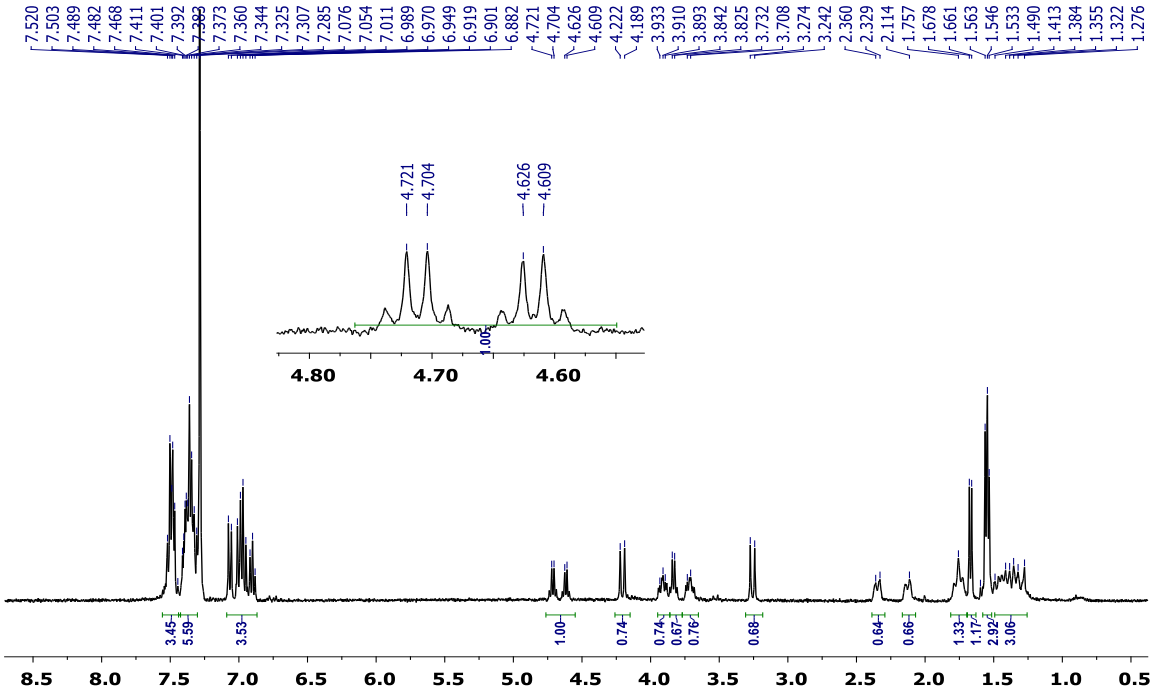


Figure 33: ^{1}H NMR spectra of **15** with (*S*,*S*,*S*)-**4**

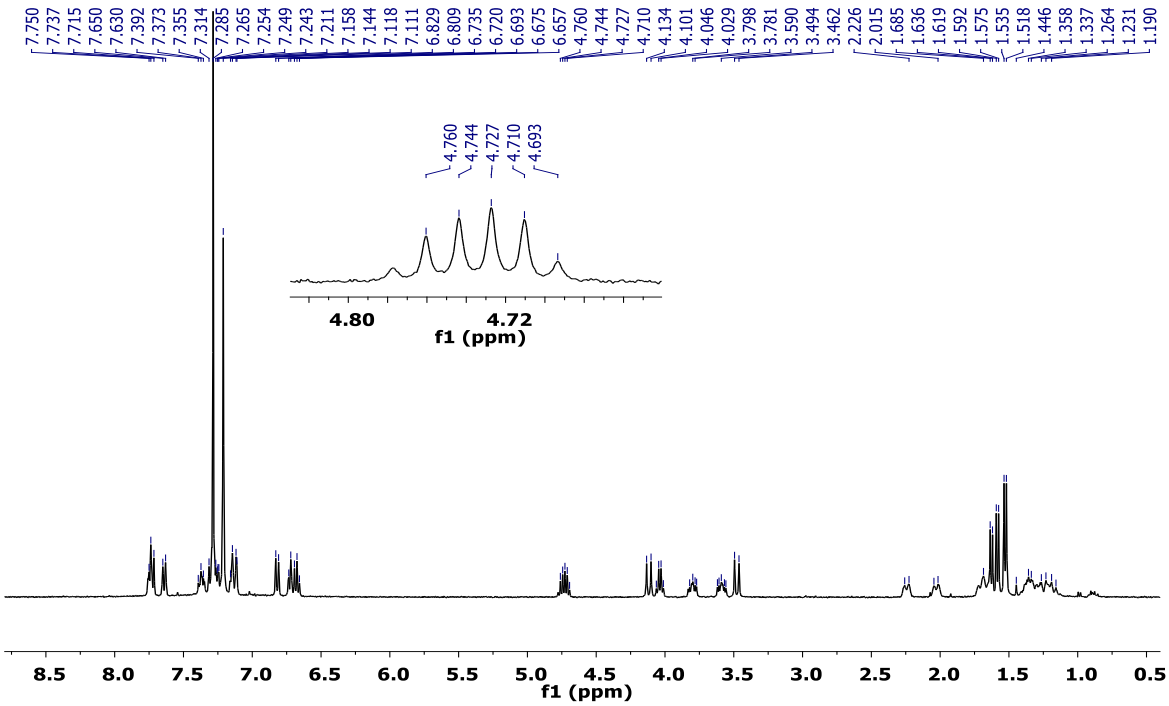


Figure 34: ^{1}H NMR spectra of **16** with (*R*,*R*,*S*)-**4**

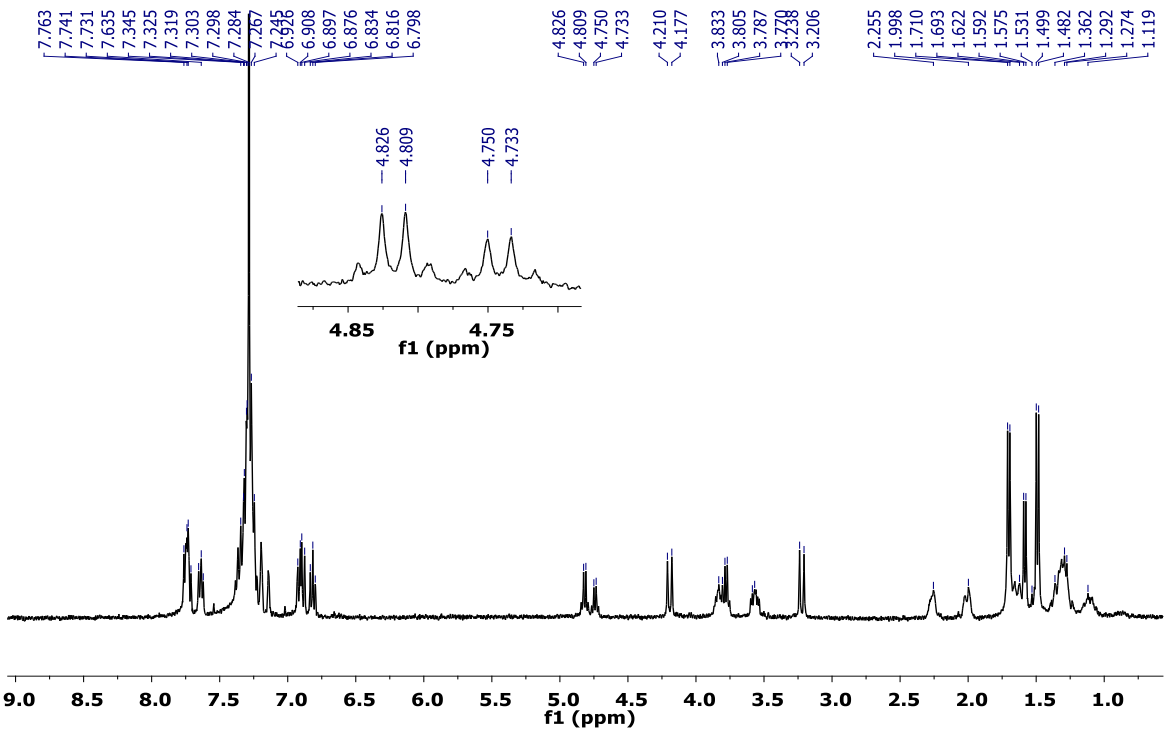


Figure 35: ^{1}H NMR spectra of **16** with (*S*,*S*,*S*)-**4**

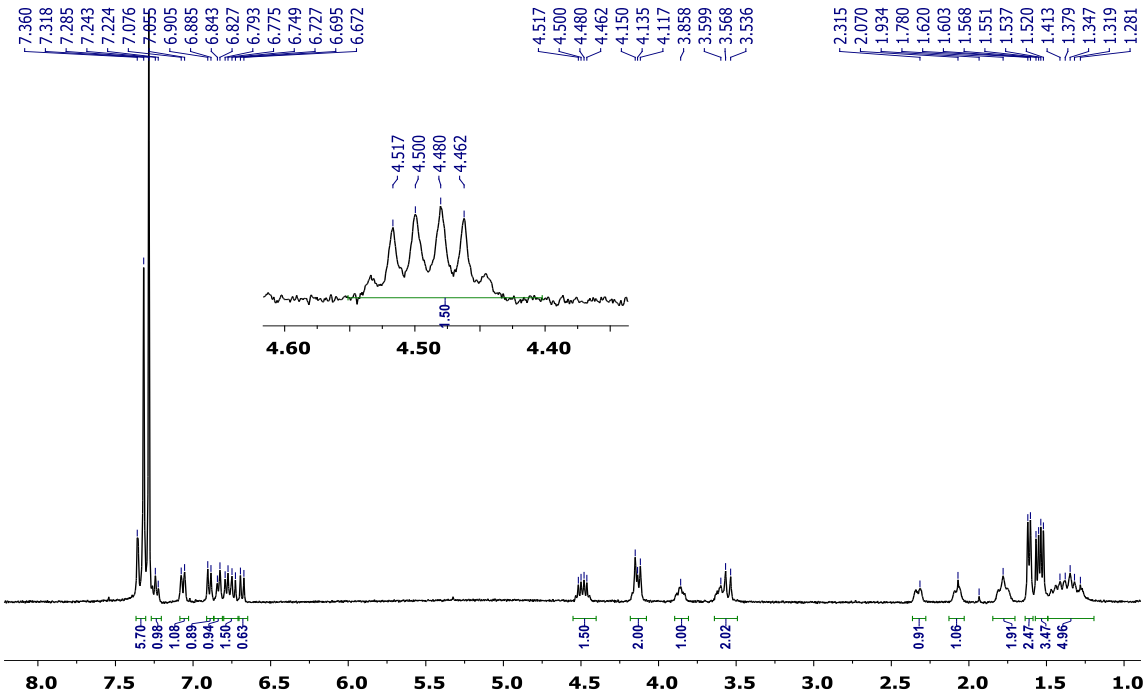


Figure 36: ^{1}H NMR spectra of **17** with (*R*,*R*,*S*)-**4**

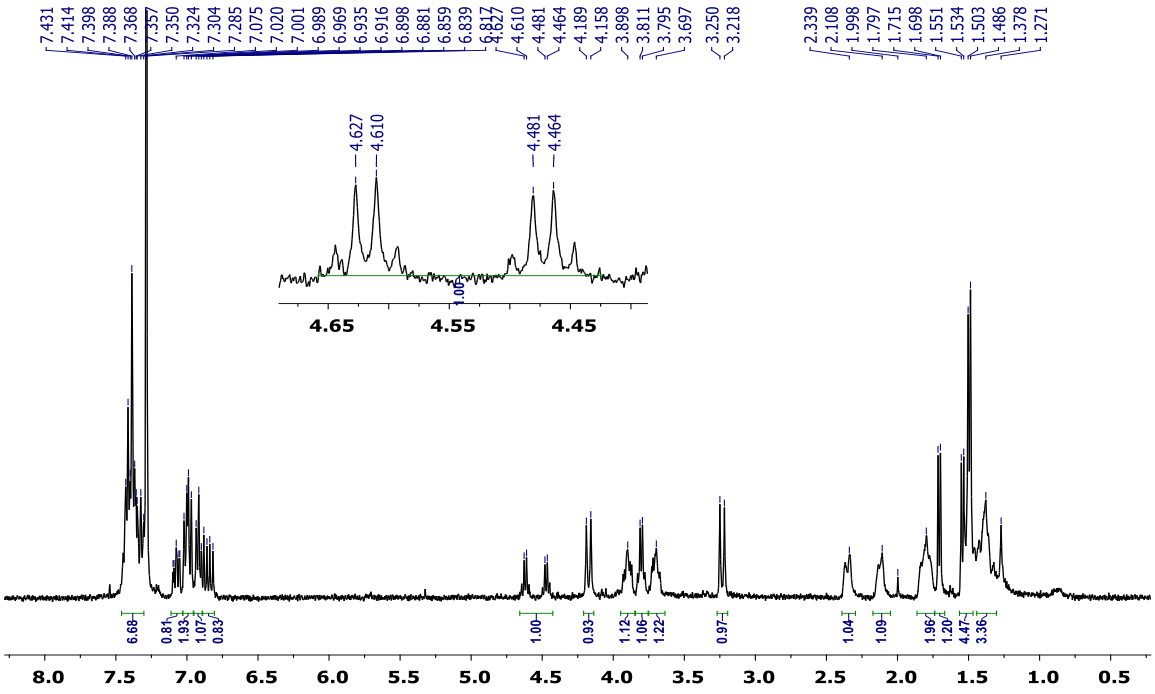


Figure 37: ^{1}H NMR spectra of **17** with (*S*,*S*,*S*)-**4**

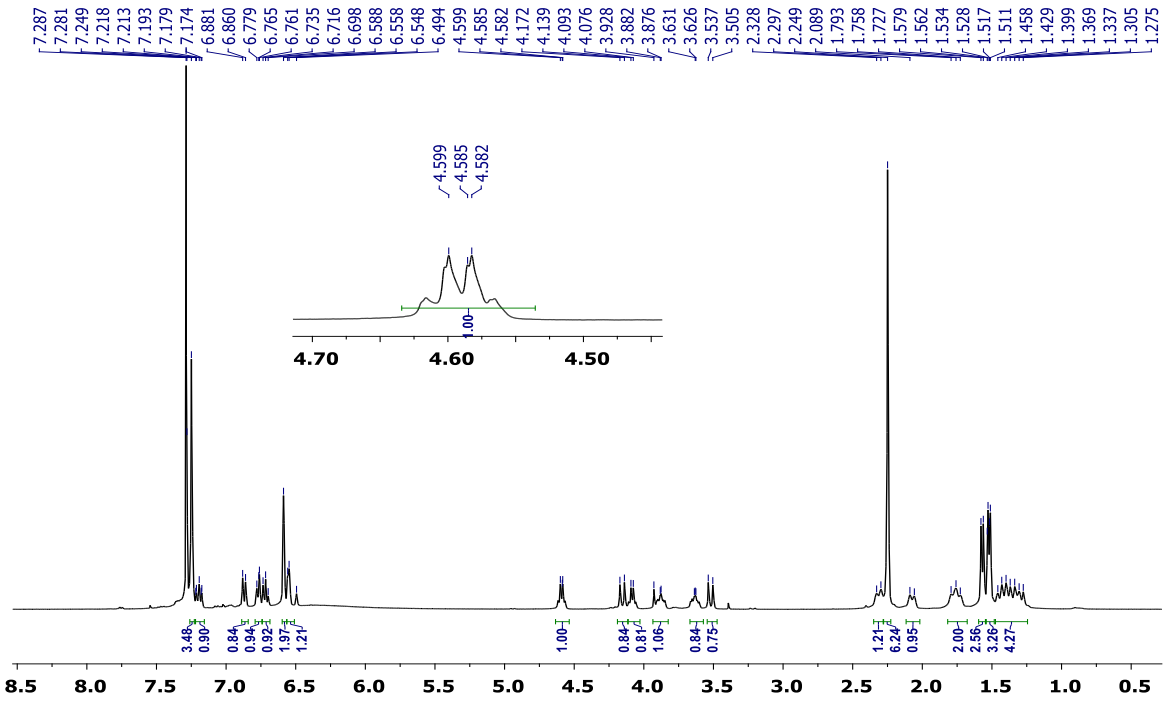


Figure 38: ^{1}H NMR spectra of **18** with (*R*,*R*,*S*)-**4**

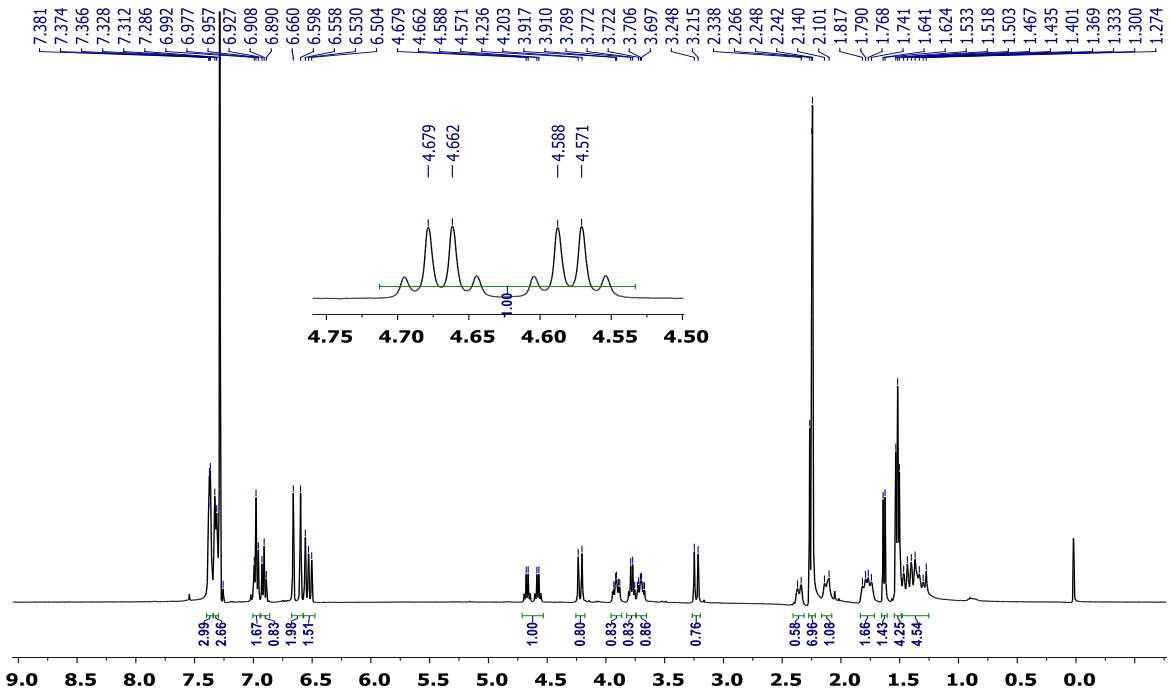


Figure 39: ^{1}H NMR spectra of **18** with (*S*,*S*,*S*)-**4**

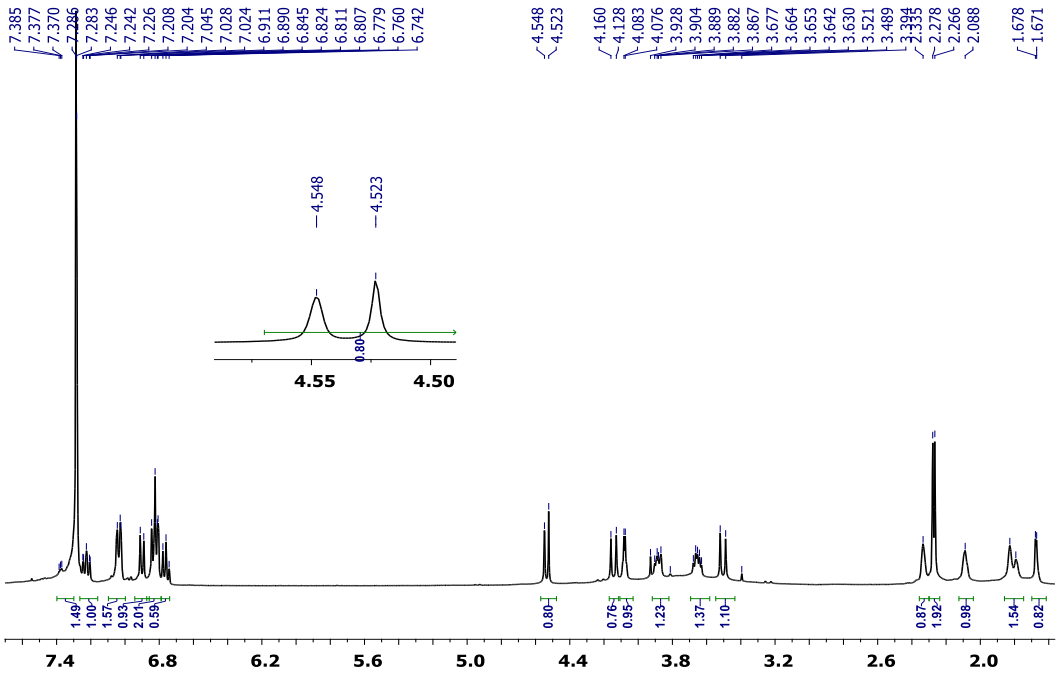


Figure 40: 1D- ^{1}H Homo-decoupled NMR spectra of **14** with (*R*,*R*,*S*)-**4**

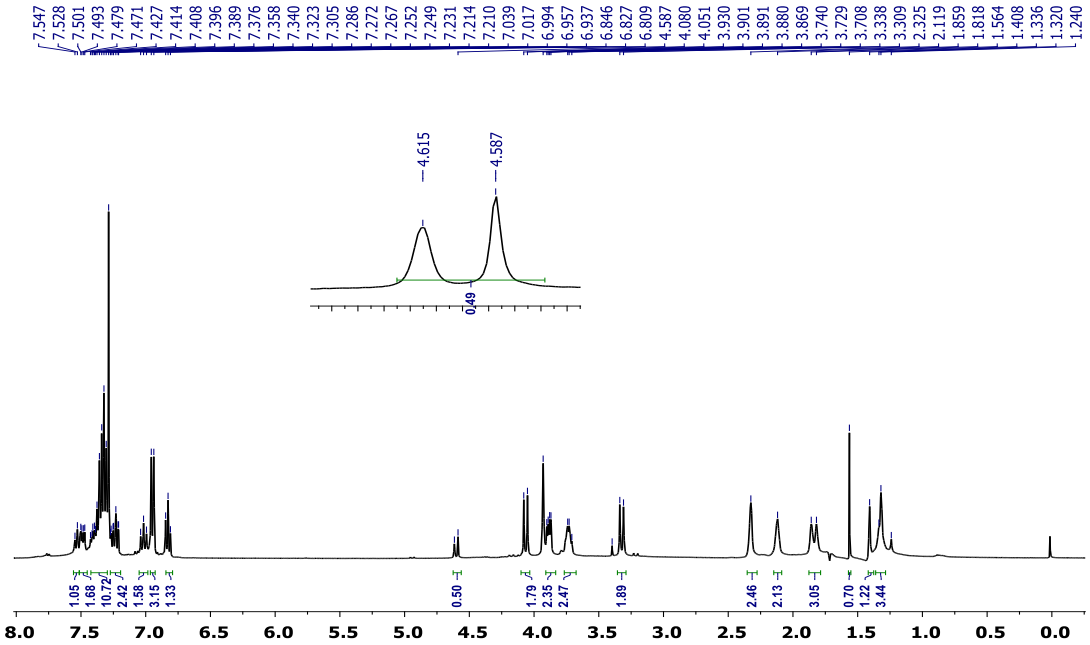


Figure 41: 1D- ^{1}H Homo-decoupled NMR spectra of **15** with (*R*,*R*,*S*)-**4**

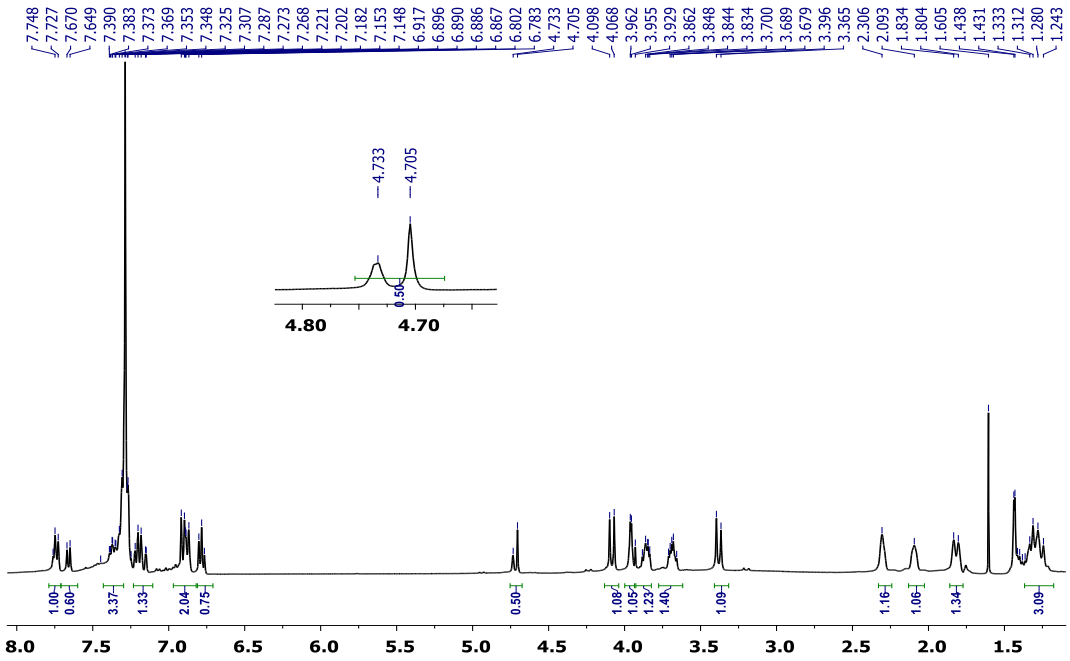


Figure 42: 1D- ^{1}H Homo-decoupled NMR spectra of **16** with (*R*,*R*,*S*)-**4**

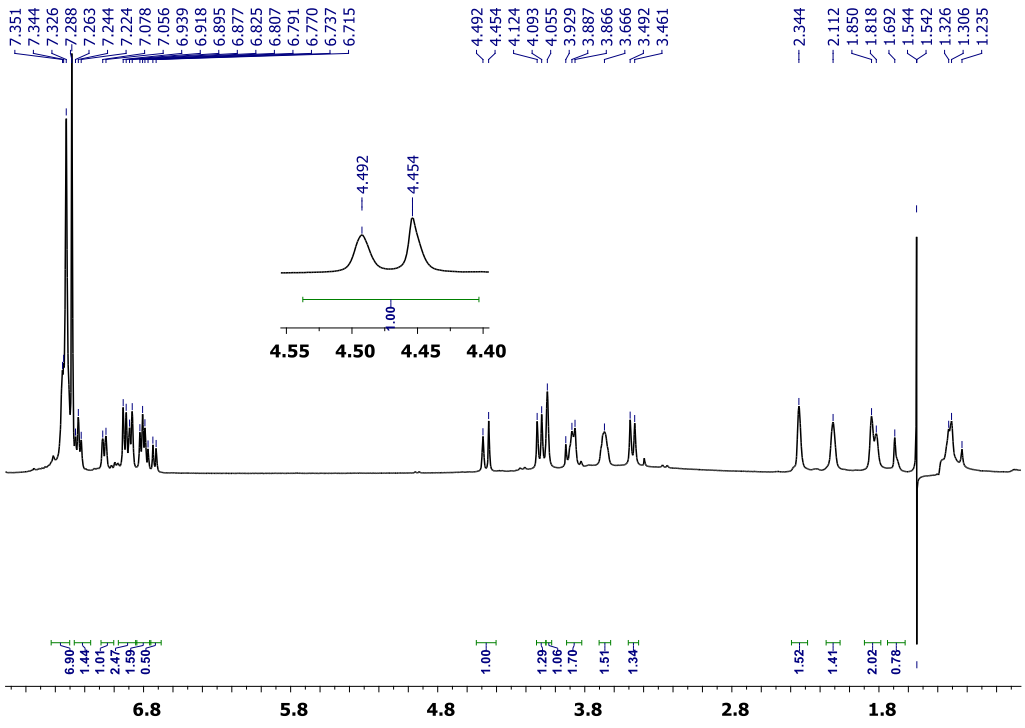


Figure 43: 1D- ^{1}H Homo-decoupled NMR spectra of **17** with (*R*,*R*,*S*)-**4**

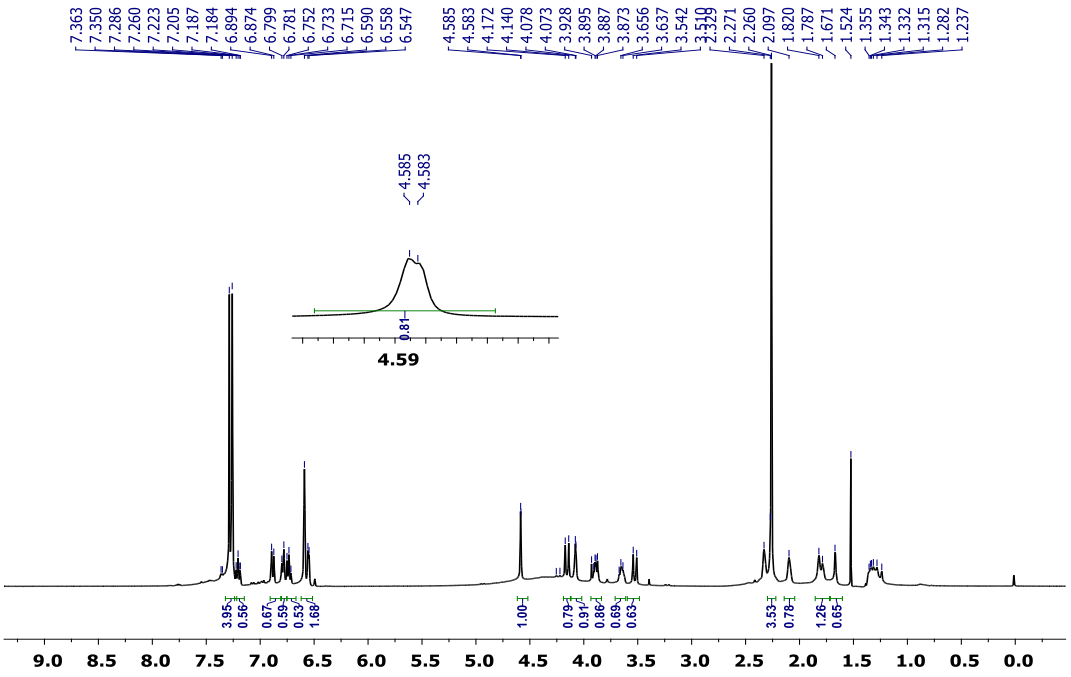


Figure 44: 1D- ^{1}H Homo-decoupled NMR spectra of **18** with (*R*,*R*,*S*)-**4**

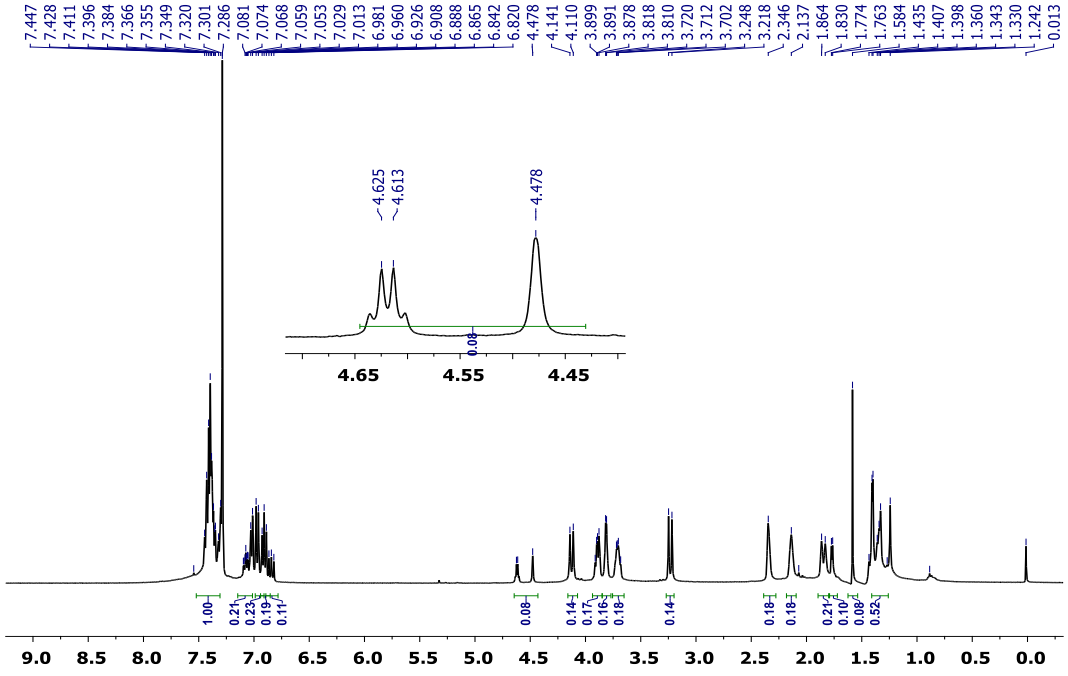


Figure 45: 1D- ^{1}H Homo-decoupled NMR spectra of **17** with (*R*,*R*,*S*)-**4**

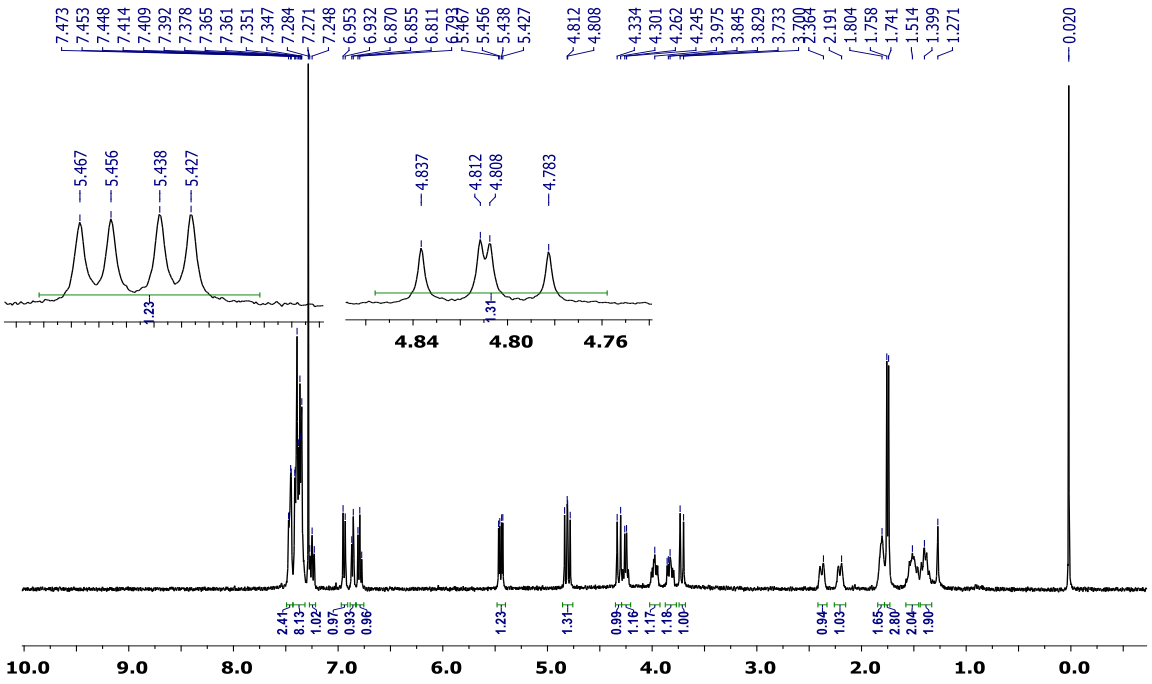


Figure 46: ^{1}H NMR spectra of **19** with (*S*,*S*,*S*)-**4**

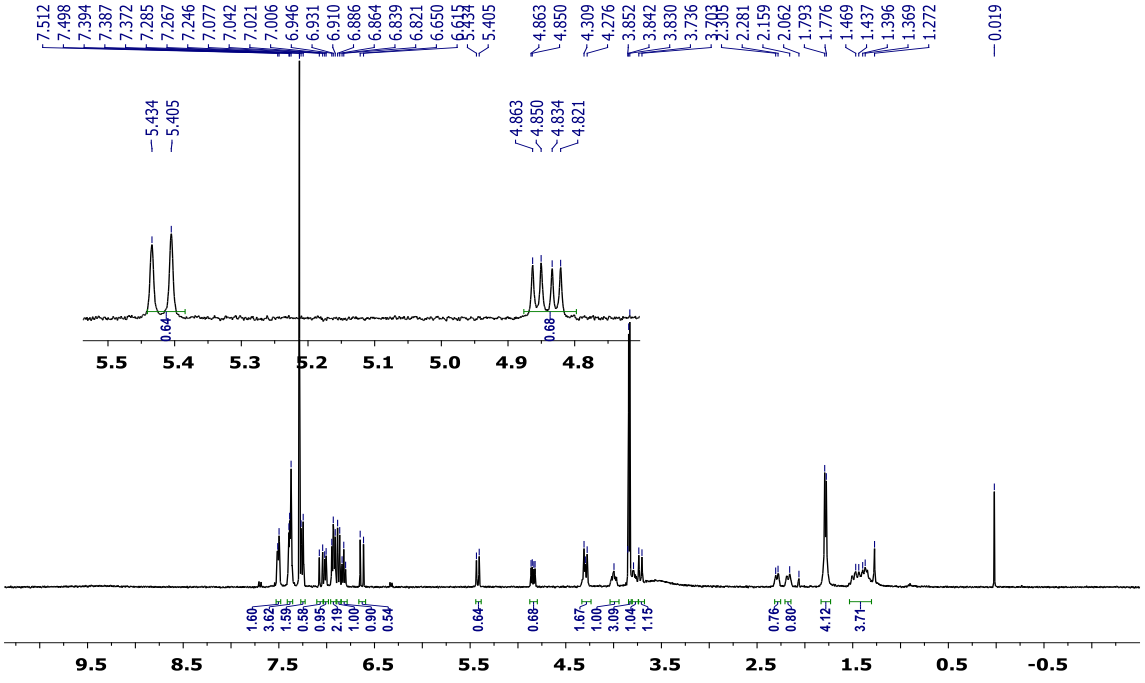


Figure 47: ^{1}H NMR spectra of **20** with (*S*,*S*,*S*)-**4**

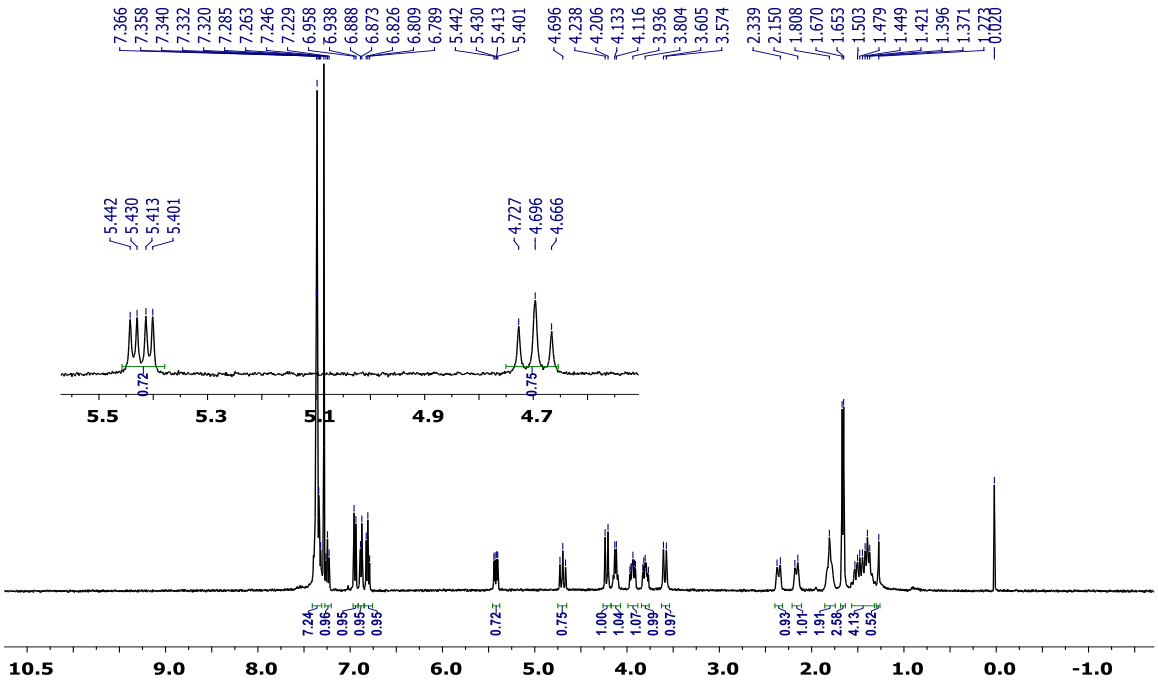


Figure 48: ^{1}H NMR spectra of **12** with (*S*,*S*,*S*)-**4**

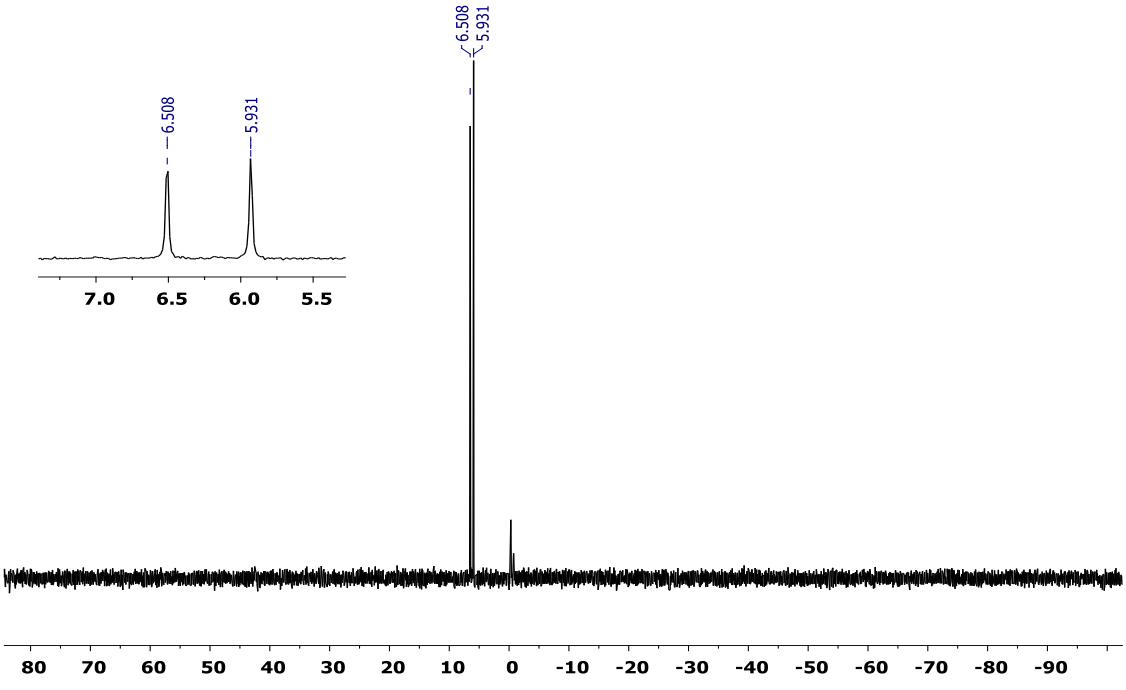


Figure 49: ^{31}P NMR spectra of **23** with (*S*,*S*,*S*)-**4**

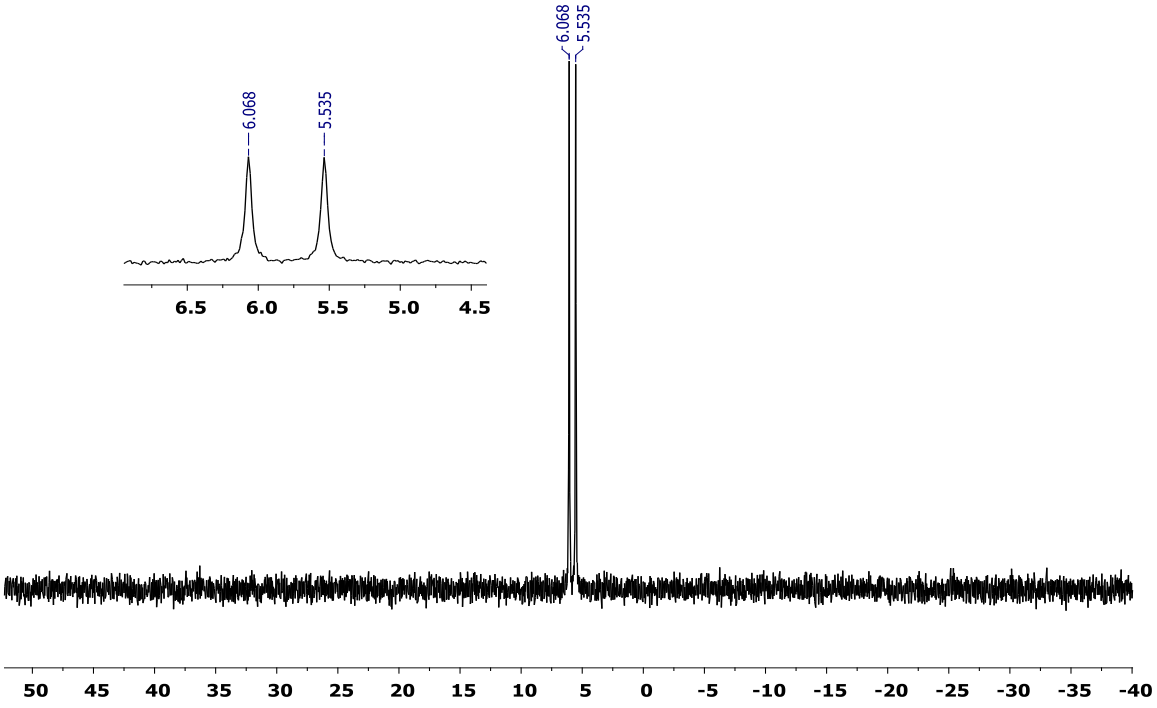


Figure 50: ^{31}P NMR spectra of **24** with (*S*,*S*,*S*)-**4**

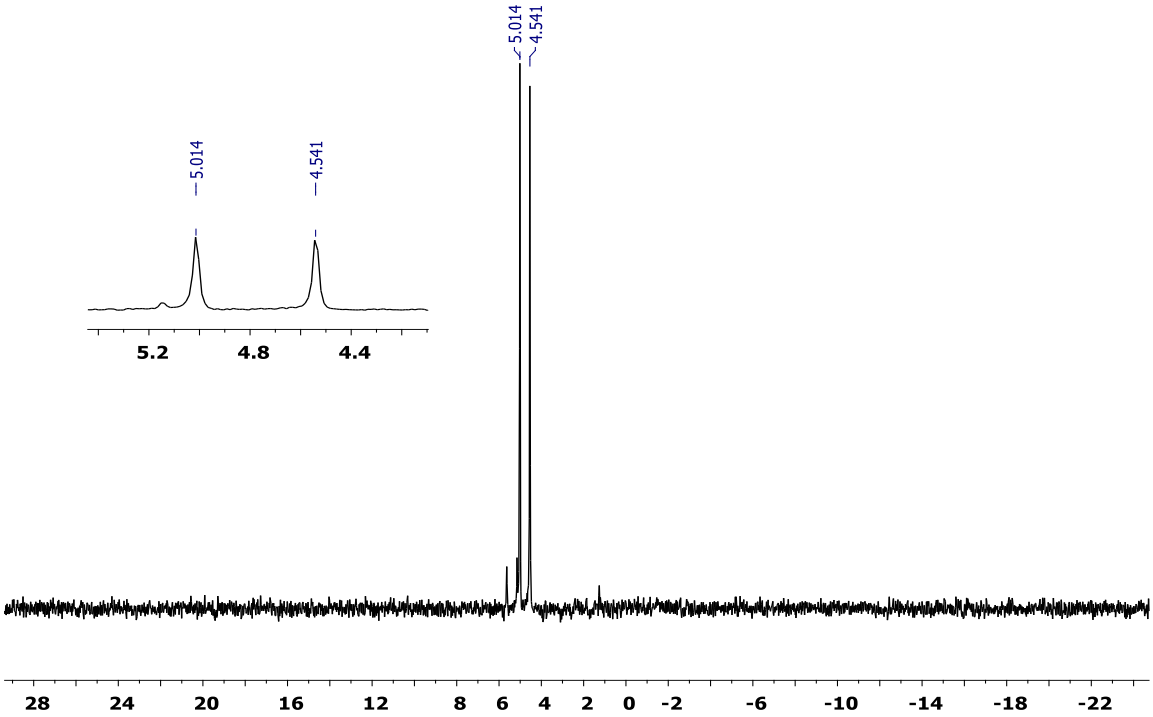


Figure 51: ^{31}P NMR spectra of **25** with (*S*,*S*,*S*)-**4**

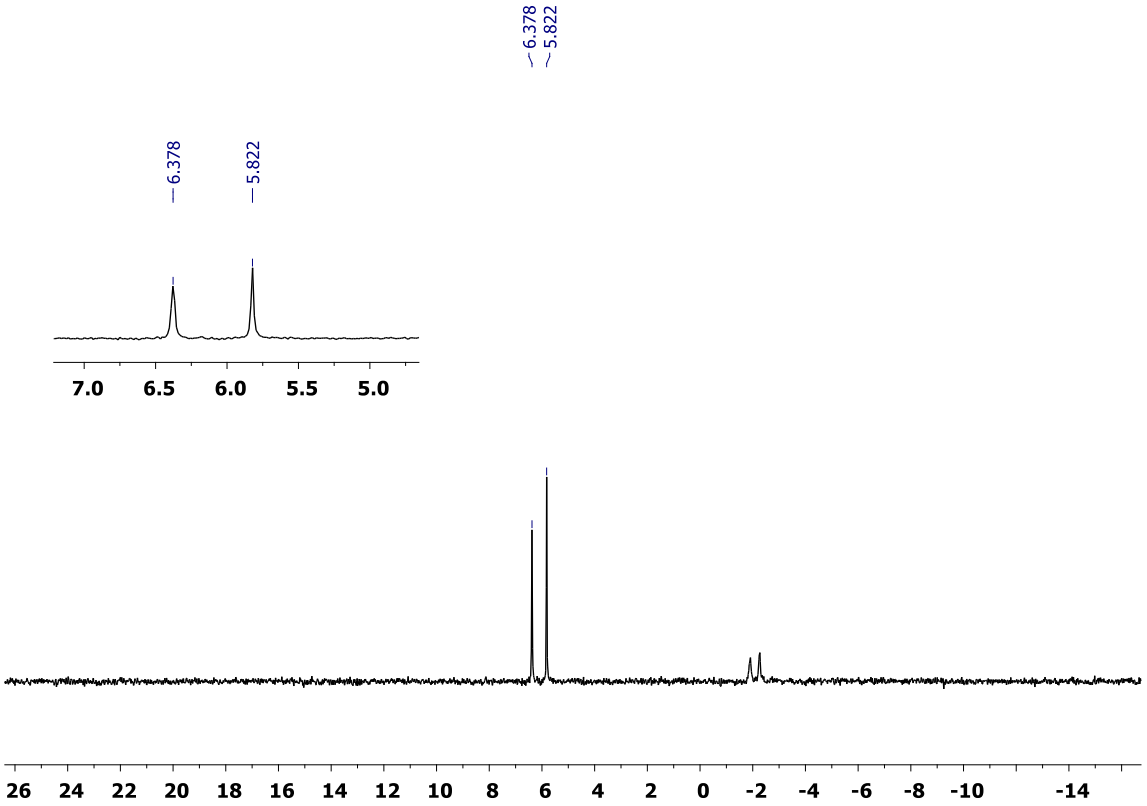


Figure 52: ^{31}P NMR spectra of **26** with (*S*,*S*,*S*)-**4**

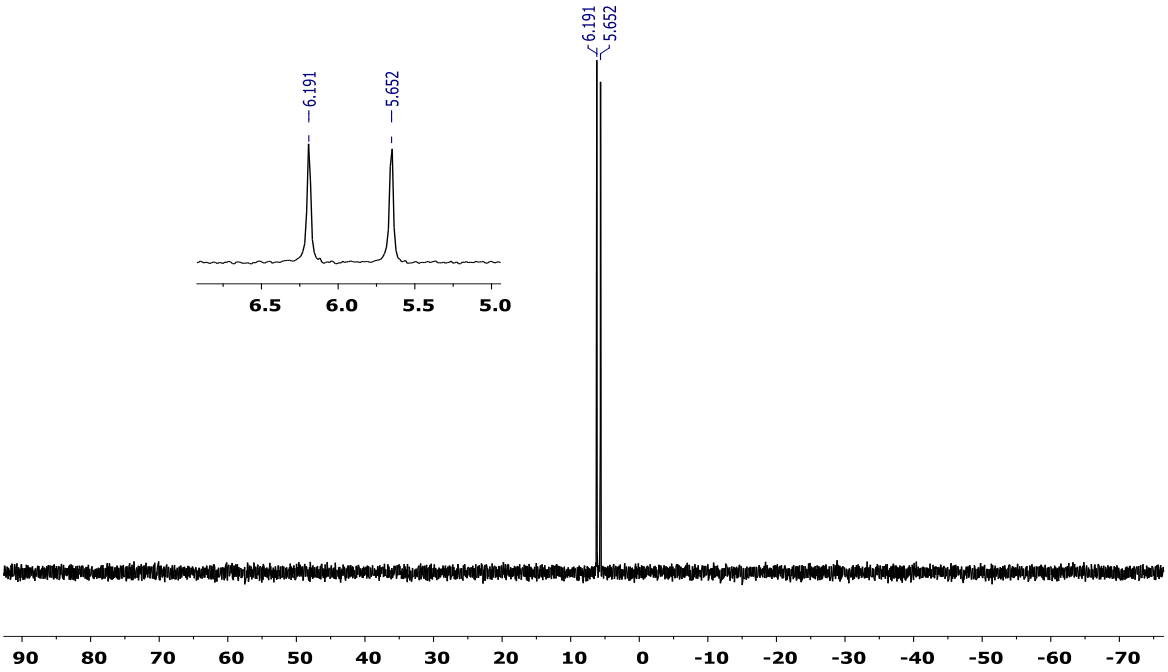


Figure 53: ^{31}P NMR spectra of **27** with (*S*,*S*,*S*)-**4**

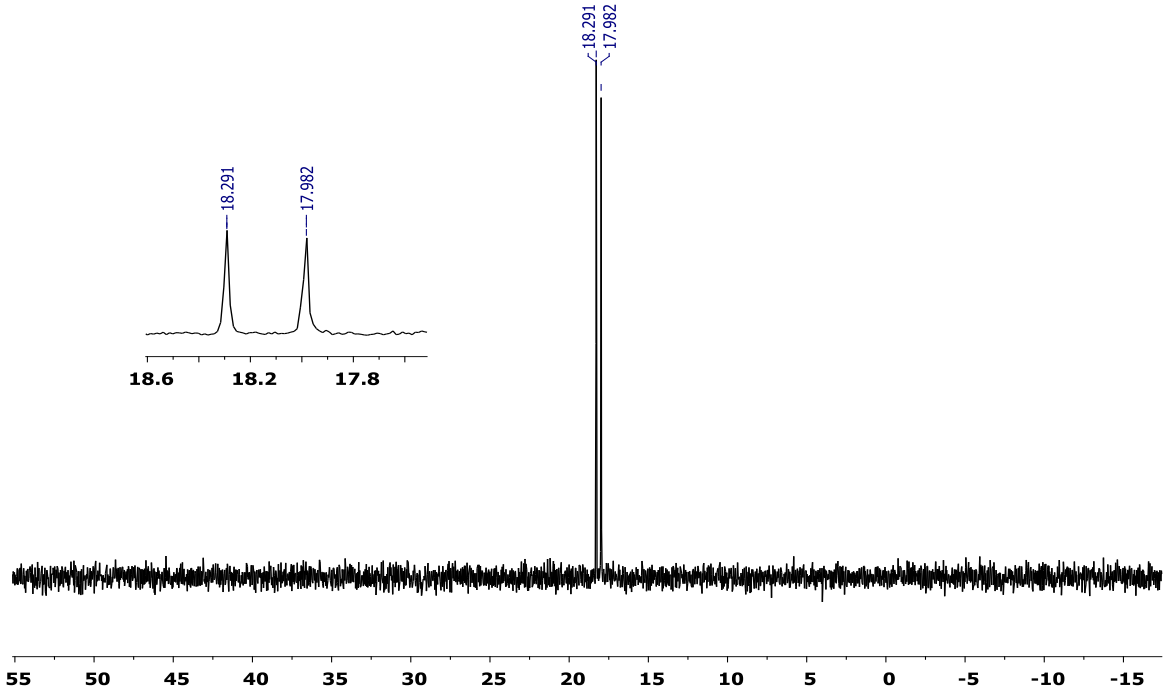


Figure 54: ^{31}P NMR spectra of **28** with (*S*,*S*,*S*)-**4**

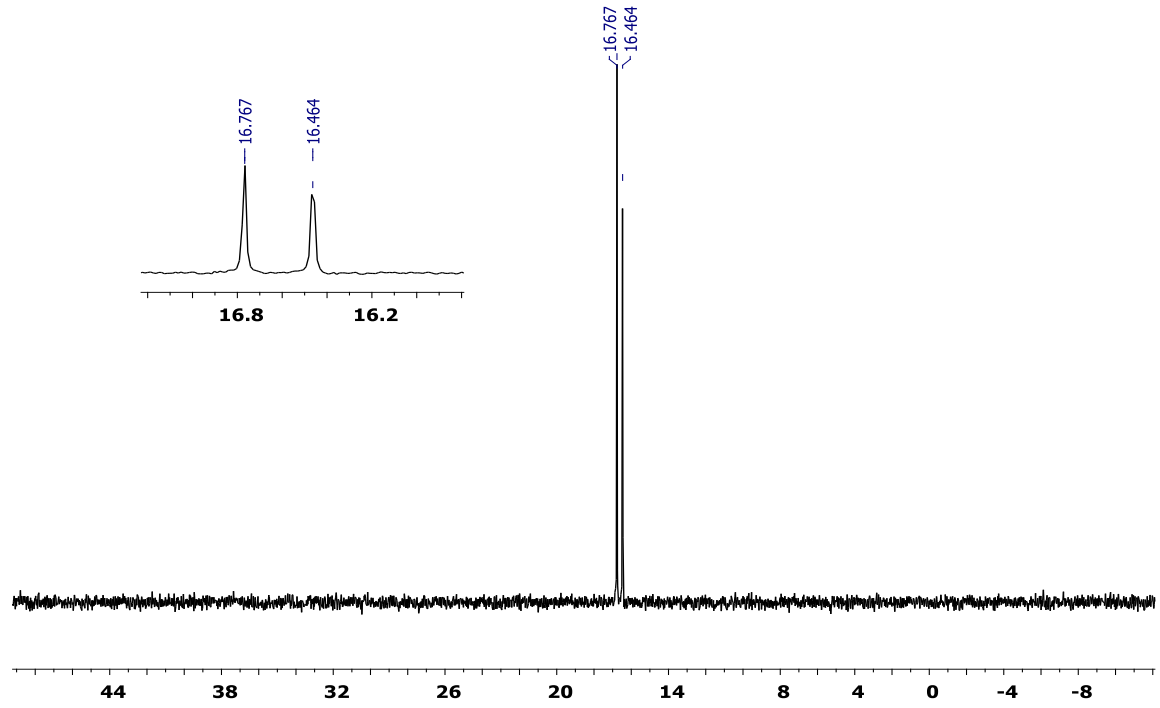


Figure 55: ^{31}P NMR spectra of **29** with (*S*,*S*,*S*)-**4**

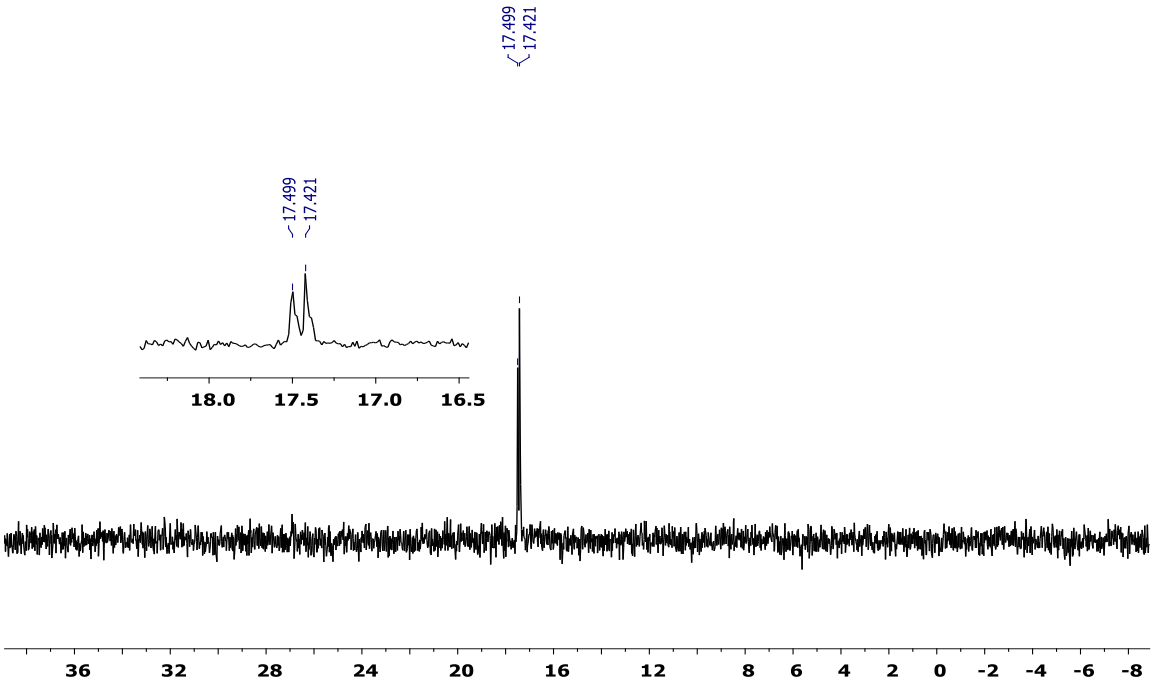


Figure 56: ^{31}P NMR spectra of **30** with (*S*,*S*,*S*)-**4**

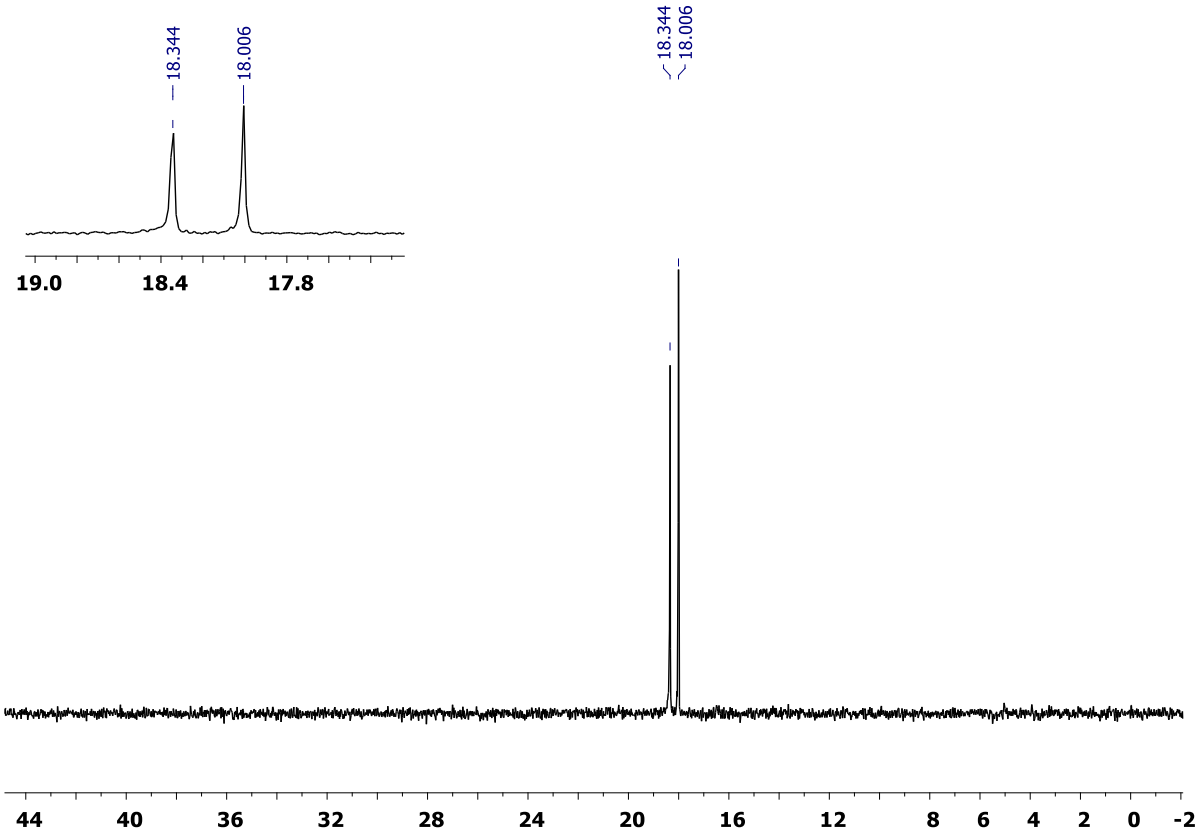


Figure 57: ^{31}P NMR spectra of **31** with (*S*,*S*,*S*)-**4**

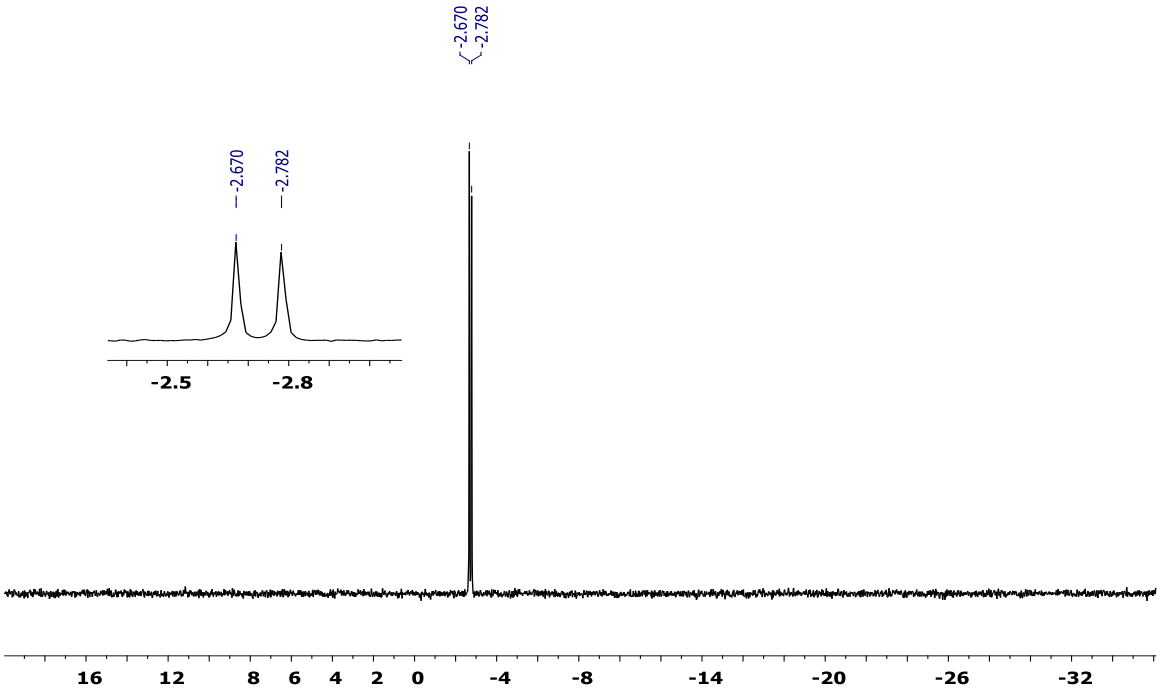


Figure 58: ^{31}P NMR spectra of **32** with (*S*,*S*,*S*)-**4**

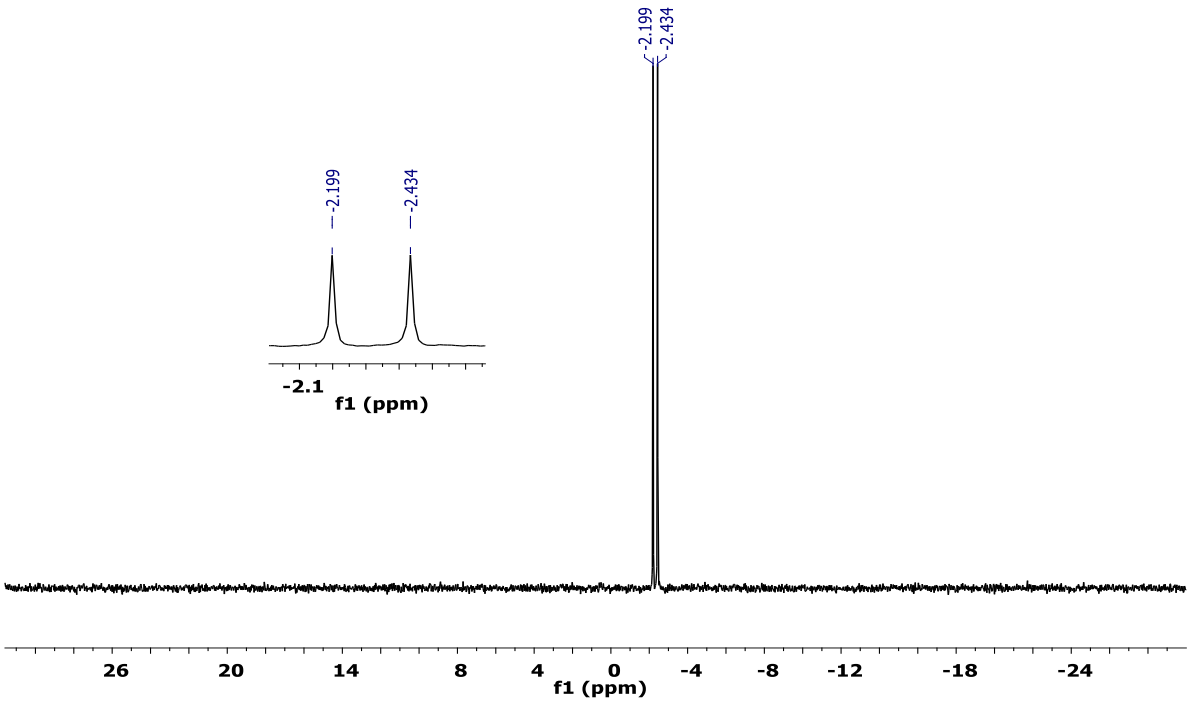


Figure 59: ^{31}P NMR spectra of **33** with (*S*,*S*,*S*)-**4**

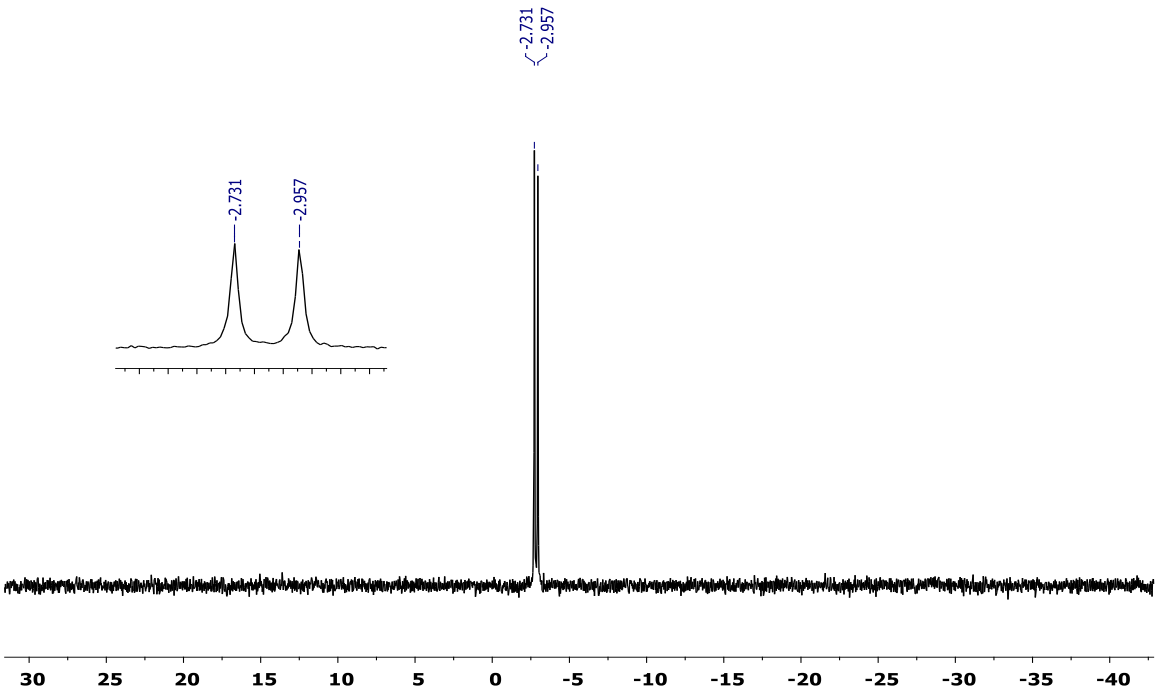


Figure 60: ^{31}P NMR spectra of **34** with (*S*,*S*,*S*)-**4**

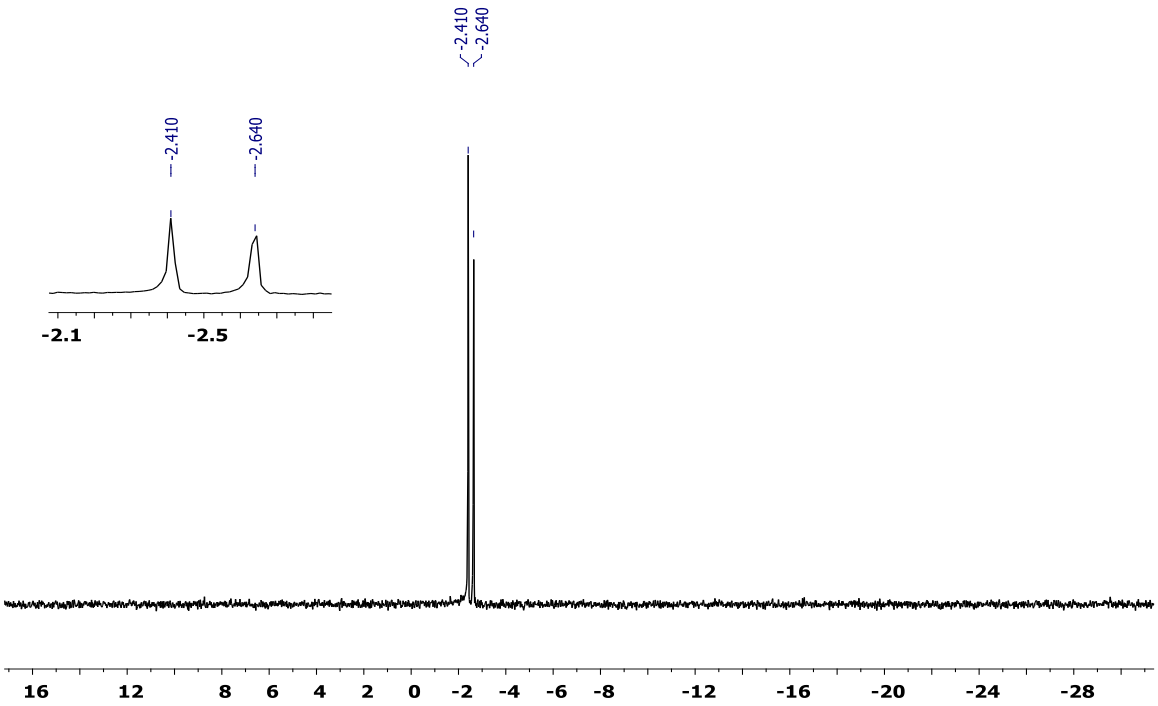


Figure 61: ^{31}P NMR spectra of **35** with (*S*,*S*,*S*)-**4**

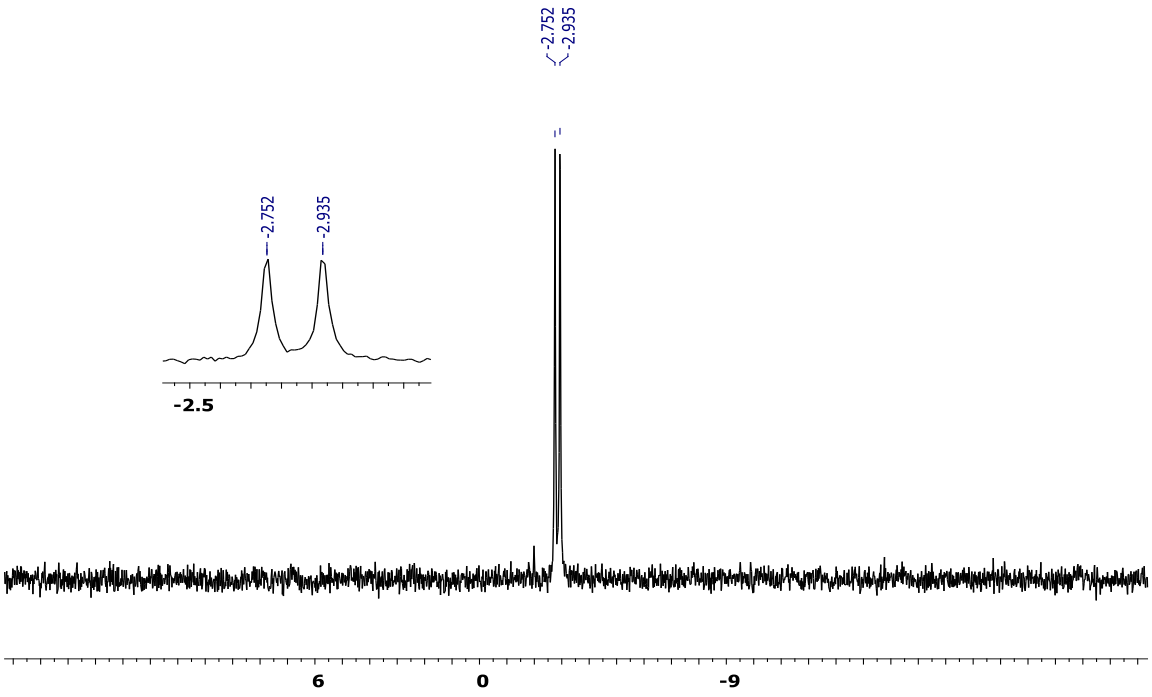


Figure 62: ^{31}P NMR spectra of **36** with (*S*,*S*,*S*)-**4**

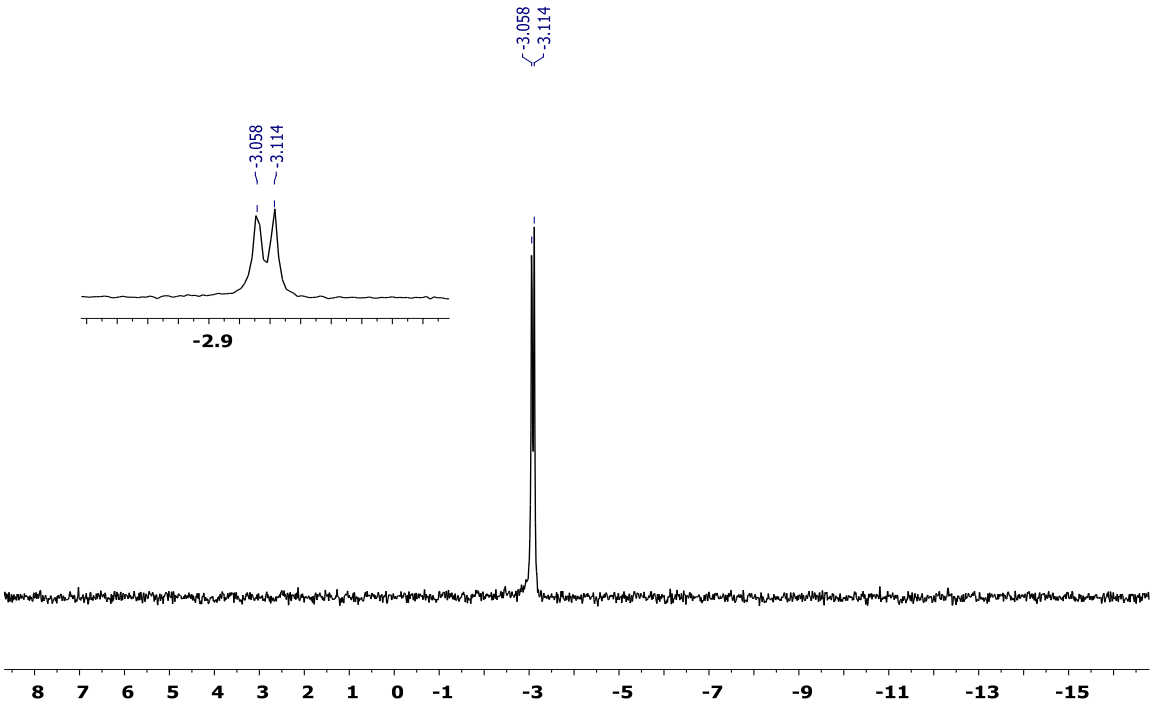


Figure 63: ^{31}P NMR spectra of **37** with (*S*,*S*,*S*)-**4**

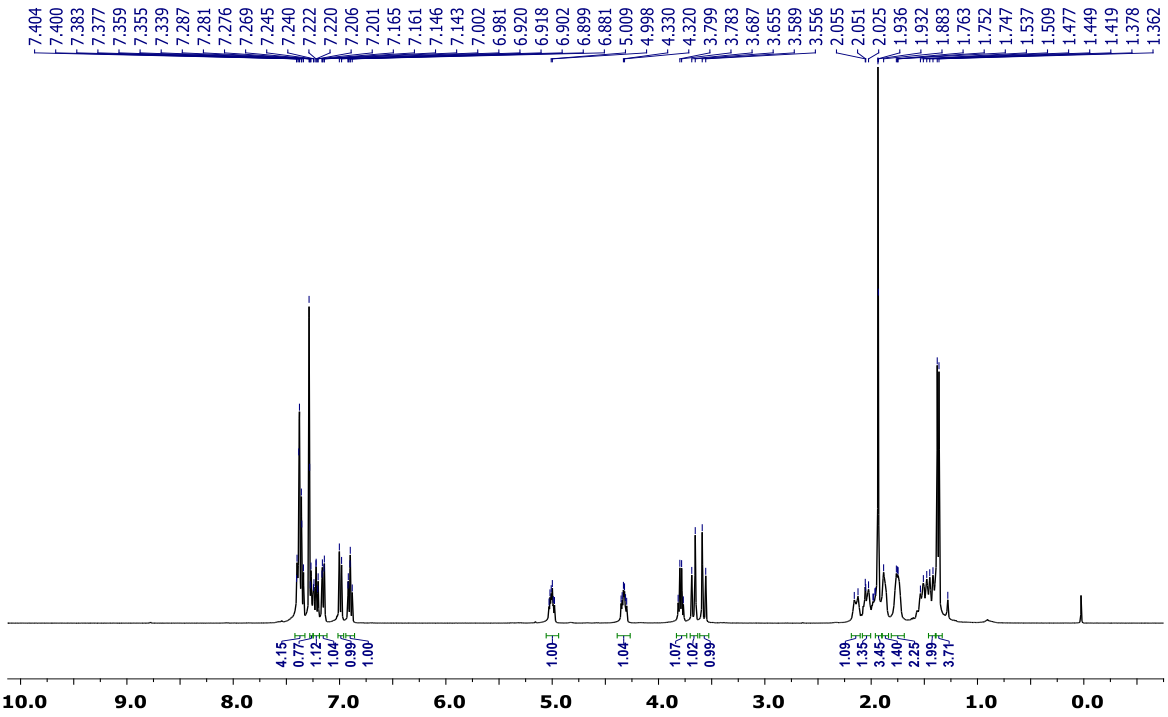


Figure 64: ^{1}H NMR of (*R*.*R*.*S*)-**23**

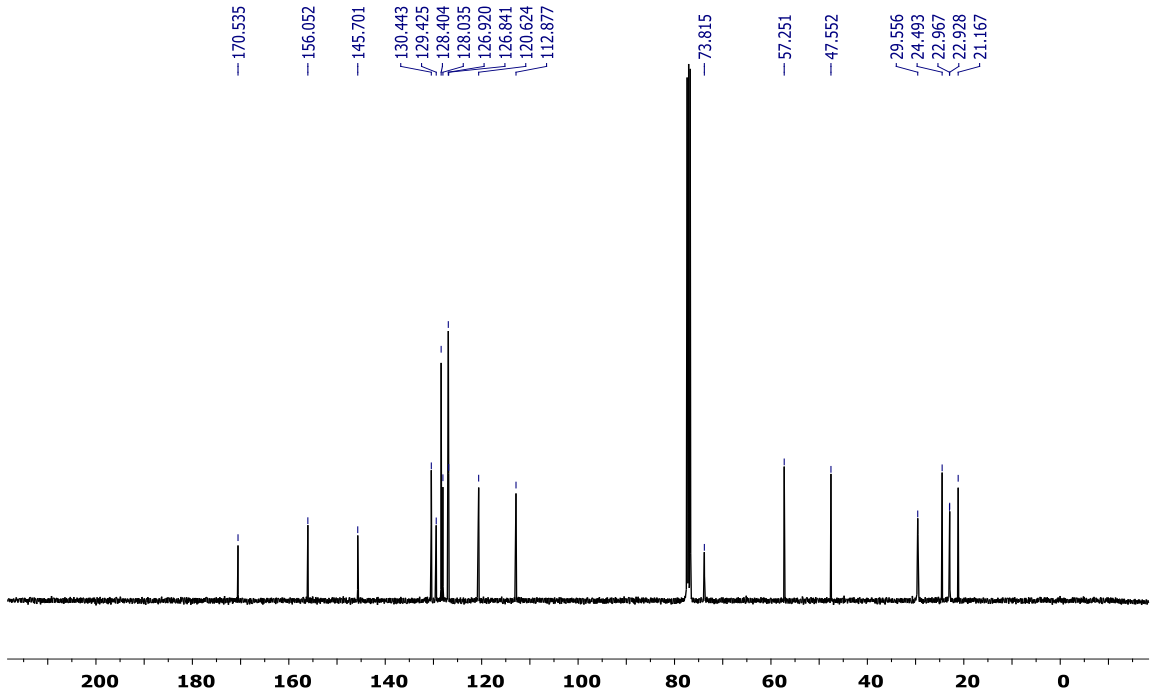


Figure 65: ^{13}CNMR of (*R*.*R*.*S*)-**23**

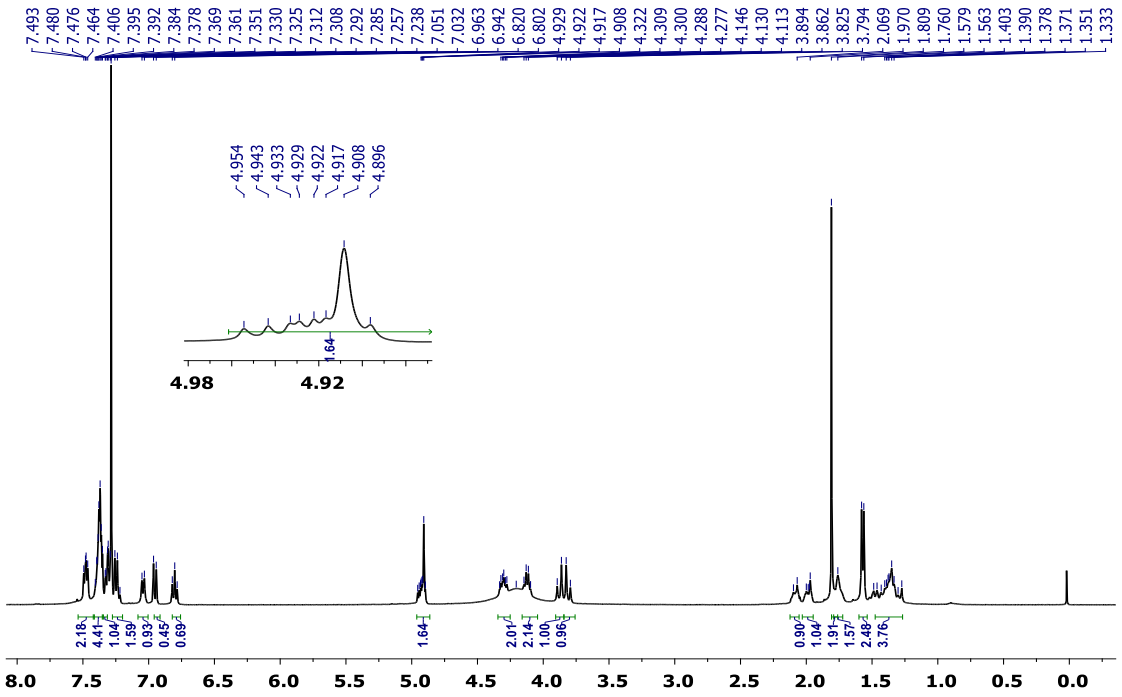


Figure 66: ^{1}H NMR of **7** with (*R*.*R*.*S*)-**23**

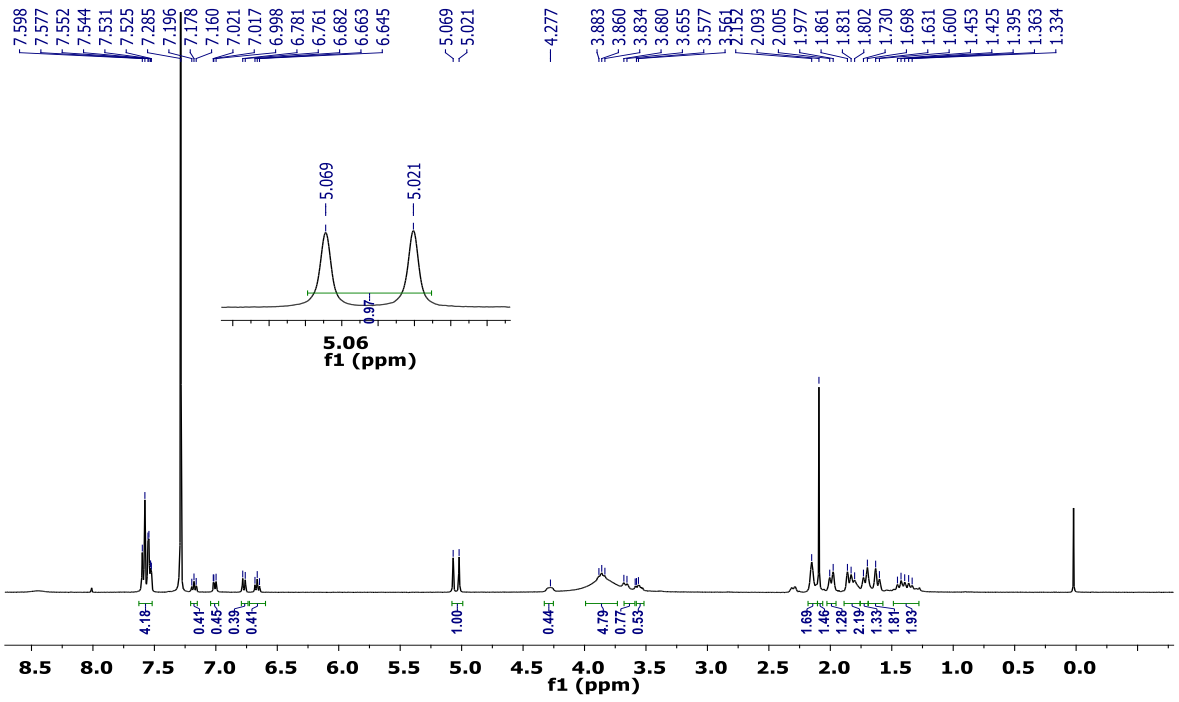


Figure 67: ^{1}H NMR of **7** with (*S*.*S*)-**6**

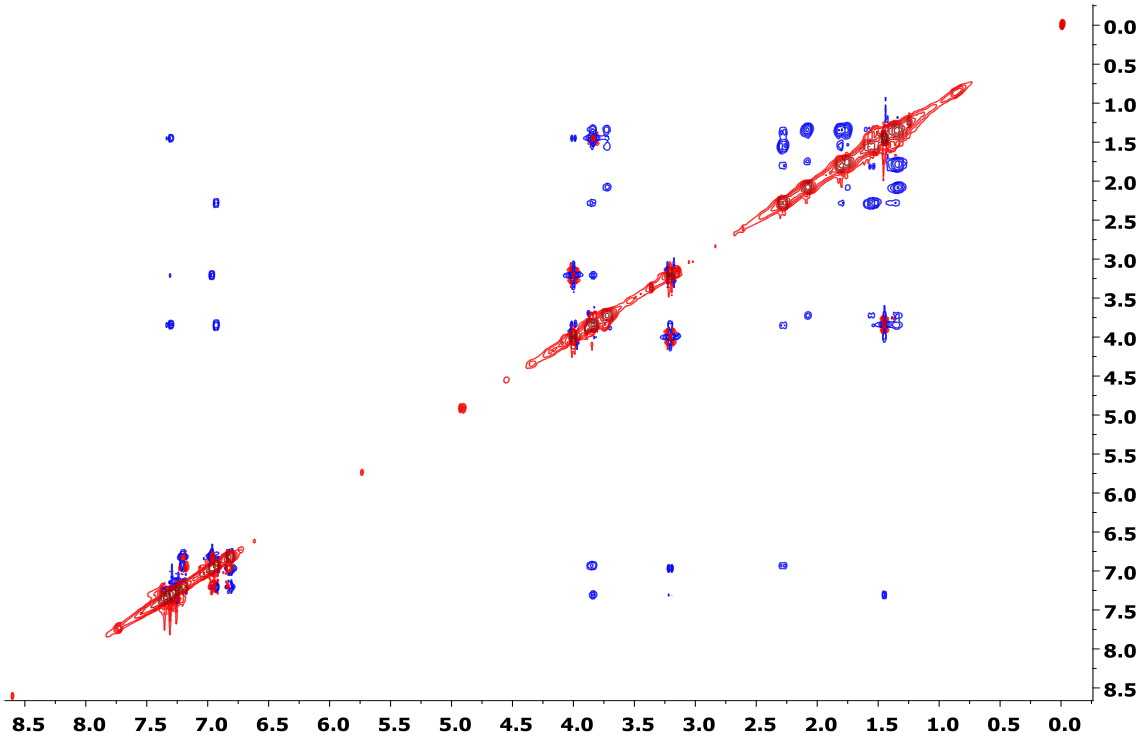


Figure 68: 2D NOESY of (*R*,*R*,*S*)-**4**

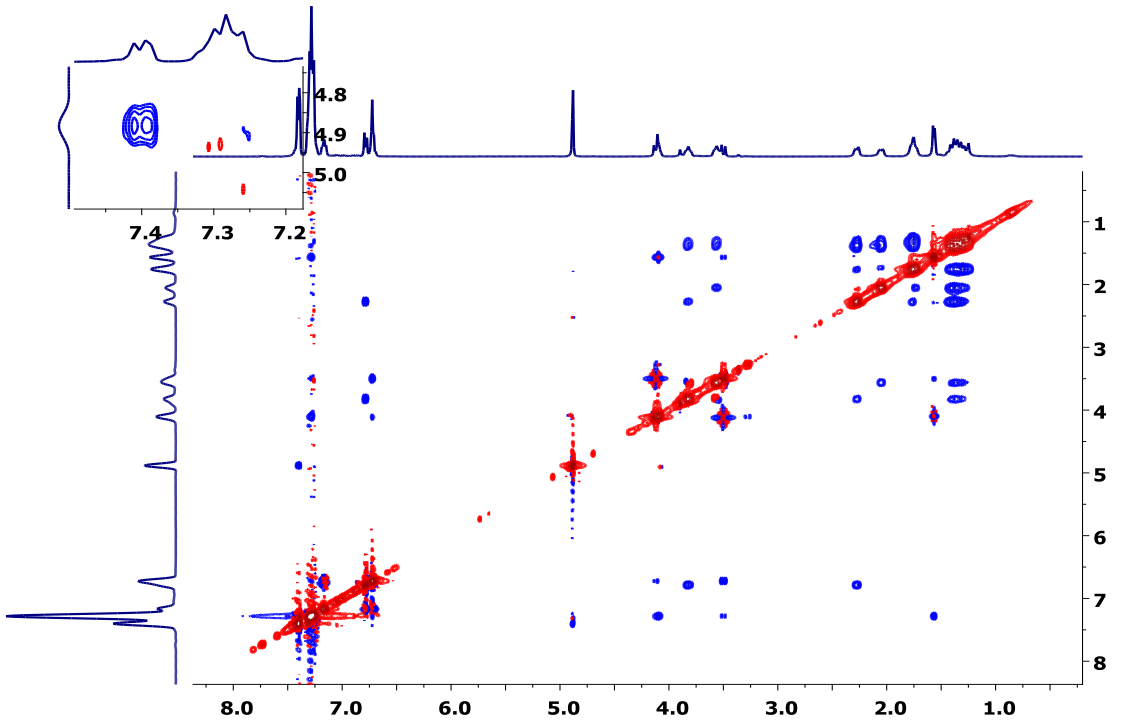


Figure 69: 2D NOESY of (*R*,*R*,*S*)-**4** with *R*-**7**

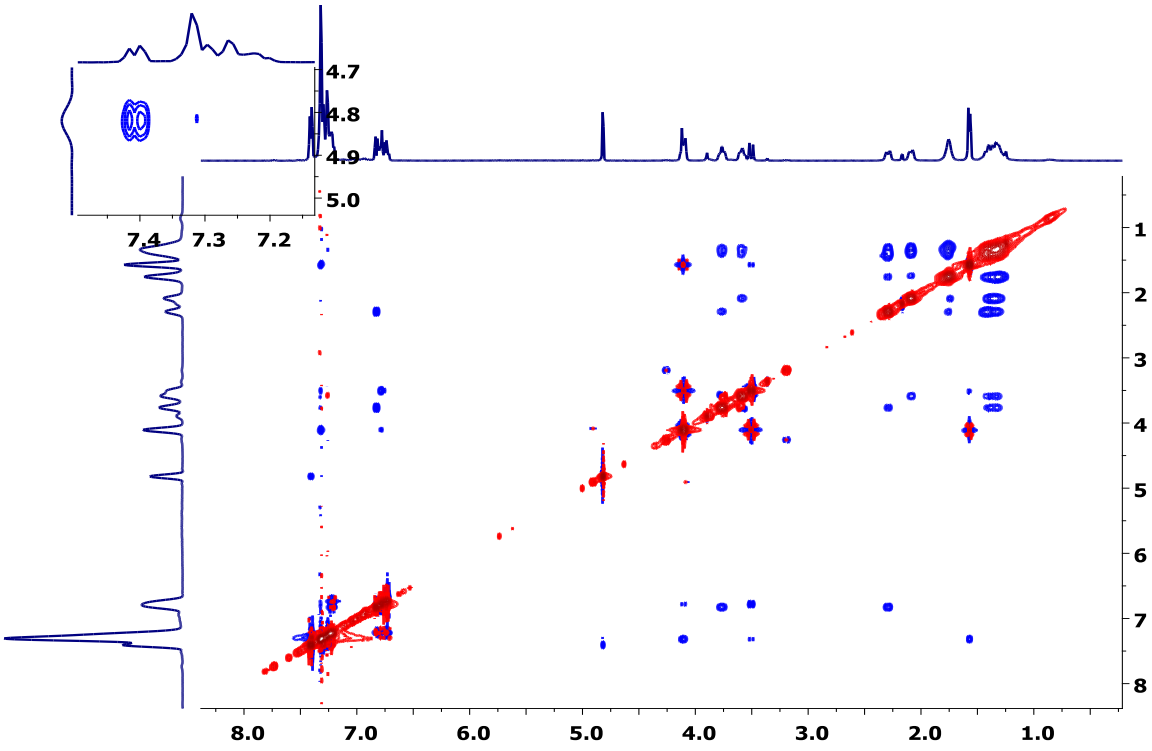


Figure 70: 2D NOESY of (*R*,*R*,*S*)-**4** with *S*-**7**

NMR experimental parameters used in the acquisitions of selective homo-decoupling ^{1}H NMR experiments:

No.	2D NOESY experiment details	Parameters
1.	Relaxation delay (D1)	1.9386 sec
2.	Number of scans (NS)	16
3.	Mixing time (D8)	0.3000001 sec
4.	Data acquisition mode (FnMODE)	states-TPPIs
5.	Spectral width (sw)	8.167 ppm
6.	Pulse program	noesygpphpp
7.	Pulse width p1	8.0000
8.	Receiver gain (rg)	101

No.	^{1}H selective homo-decoupling experiment details	Parameters
1.	Relaxation delay (D1)	3.000
2.	Number of scans (NS)	32
3.	Spectral width (sw)	8196.7
4.	Pulse program	zghd.2
5.	Pulse width p1	8.0000
6.	Receiver gain (rg)	101
7.	Power level PL24	30.34dB
8.	Acquisition time	1.9988

Single-crystal X-ray diffraction for (*S*,*S*,*S*)-4 + D tartaric acid:

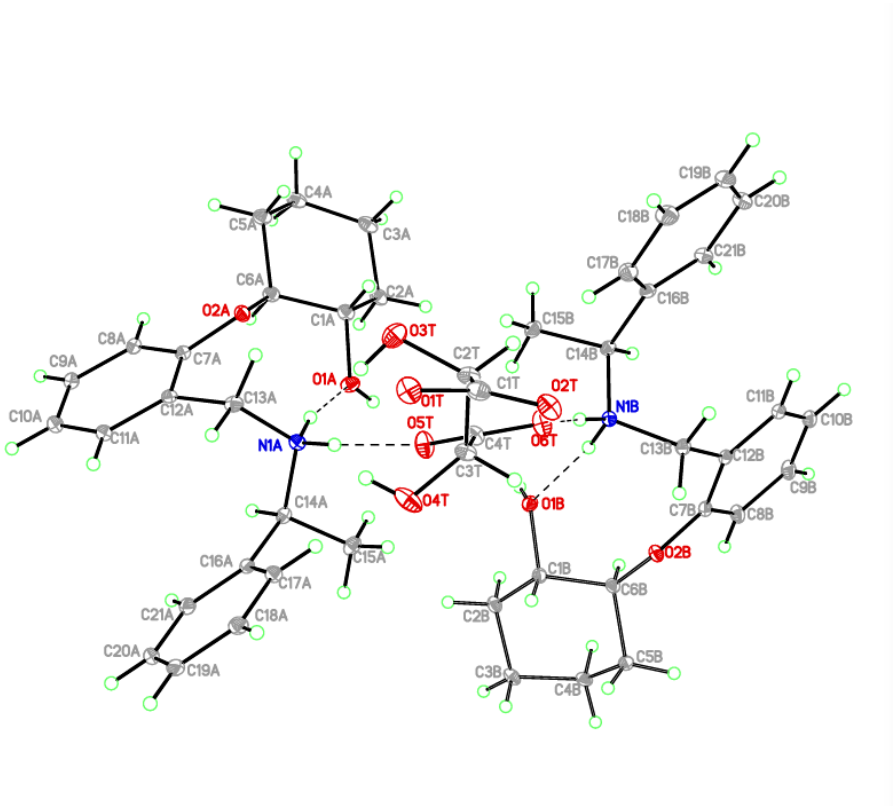


Figure 71: ORTEP diagram of salt of (S,S,S)-4 and D-tartaric acid (CCDC2352208)

Table 1. Crystal data and structure refinement for salt of (*S*,*S*,*S*)-**4** and D-tartaric acid (CCDC2352208).

Identification code	Salt of (*S*,*S*,*S*)-**4** and D-tartaric acid (CCDC2352208)	
Empirical formula	C46 H60 N2 O10	
Formula weight	800.96	
Temperature	296(2) K	
Wavelength	1.54184 Å	
Crystal system	Hexagonal	
Space group	P 61	
Unit cell dimensions	a = 10.99230(10) Å	α= 90°.
	b = 10.99230(10) Å	β= 90°.
	c = 61.8008(6) Å	γ = 120°.
Volume	6466.98(13) $Å^3$	
Z	6	
Density (calculated)	1.234 Mg/m^3	
Absorption coefficient	0.701 mm^{-1}	
F(000)	2580	
Crystal size	0.29 x 0.20 x 0.11 mm^3	

Theta range for data collection	2.860 to 76.358°.
Index ranges	-13<=h<=13, -13<=k<=11, -45<=l<=77
Reflections collected	83354
Independent reflections	7605 [R(int) = 0.0412]
Completeness to theta = 67.684°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.74160
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7605 / 1130 / 768
Goodness-of-fit on F^2	1.065
Final R indices [I>2sigma(I)]	R1 = 0.0559, wR2 = 0.1718
R indices (all data)	R1 = 0.0594, wR2 = 0.1771
Absolute structure parameter	-0.04(8)
Extinction coefficient	n/a
Largest diff. peak and hole	0.481 and -0.394 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for salt of (*S,S,S*)-**4** and D-tartaric acid (CCDC2352208).
U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(2B)	2537(3)	1991(3)	5454(1)	64(1)
N(1B)	5282(3)	1892(3)	5461(1)	52(1)
O(1B)	3184(9)	719(11)	5111(2)	59(2)
C(1B)	2163(12)	1133(17)	5099(2)	60(2)
C(2B)	1155(11)	398(12)	4914(2)	66(2)
C(3B)	195(11)	957(13)	4878(2)	72(2)
C(4B)	-508(11)	1052(13)	5078(2)	69(2)
C(5B)	292(10)	1427(12)	5294(2)	66(2)
C(6B)	1434(13)	1032(16)	5308(2)	60(2)
O(1D)	3040(9)	531(11)	5163(2)	65(2)
C(1D)	2140(12)	1062(15)	5101(2)	60(1)
C(2D)	977(10)	100(12)	4944(2)	67(2)
C(3D)	-87(10)	586(12)	4904(2)	74(2)
C(4D)	-760(9)	607(11)	5120(2)	70(2)
C(5D)	595(9)	1903(10)	5246(2)	67(1)
C(6D)	1434(12)	1170(14)	5307(2)	60(2)
C(7B)	2506(2)	1545(3)	5659(1)	59(1)
C(8B)	1282(2)	721(3)	5776(1)	76(1)
C(9B)	1361(3)	393(3)	5991(1)	84(1)
C(10B)	2662(3)	888(3)	6089(1)	81(1)
C(11B)	3886(2)	1712(3)	5972(1)	69(1)
C(12B)	3808(2)	2040(2)	5757(1)	55(1)
C(13B)	5117(4)	2826(3)	5621(1)	59(1)
C(14B)	5435(3)	724(3)	5559(1)	55(1)
C(15B)	5550(5)	-141(5)	5378(1)	78(1)
C(16B)	6666(2)	1299(3)	5717(1)	58(1)
C(17B)	8021(2)	2271(3)	5651(1)	79(1)
C(18B)	9124(2)	2763(4)	5798(1)	100(2)
C(19B)	8873(3)	2283(4)	6011(1)	99(2)
C(20B)	7518(4)	1311(4)	6076(1)	92(1)

C(21B)	6415(2)	819(3)	5929(1)	71(1)
N(1A)	6421(3)	1004(3)	4566(1)	57(1)
O(2A)	6788(3)	-1546(3)	4571(1)	67(1)
O(1A)	4737(9)	-1516(8)	4796(2)	76(2)
C(1A)	5350(12)	-2314(10)	4877(2)	68(2)
C(2A)	4238(11)	-3610(10)	5006(2)	77(2)
C(3A)	4868(12)	-4518(12)	5071(2)	84(2)
C(4A)	5582(12)	-4861(10)	4886(2)	83(2)
C(5A)	6628(11)	-3552(10)	4755(2)	76(2)
C(6A)	5815(16)	-2815(13)	4682(2)	67(1)
O(1C)	5086(10)	-1316(8)	4869(2)	67(2)
C(1C)	5566(14)	-2293(12)	4897(2)	71(2)
C(2C)	4678(13)	-3486(11)	5053(2)	78(2)
C(3C)	5295(14)	-4468(12)	5073(2)	84(2)
C(4C)	5111(14)	-5148(11)	4855(2)	81(2)
C(5C)	6183(13)	-3926(11)	4711(2)	76(2)
C(6C)	5763(19)	-2808(15)	4682(3)	67(2)
C(7A)	6610(6)	-1476(6)	4355(1)	64(1)
C(8A)	6103(7)	-2635(5)	4218(1)	69(1)
C(9A)	6119(8)	-2456(6)	3996(1)	72(1)
C(10A)	6642(8)	-1119(8)	3909(1)	75(1)
C(11A)	7149(7)	40(6)	4045(1)	71(1)
C(12A)	7133(6)	-139(5)	4268(1)	61(1)
C(7C)	6824(10)	-1372(9)	4355(1)	59(2)
C(8C)	6505(11)	-2375(8)	4195(2)	71(2)
C(9C)	6697(13)	-1982(11)	3978(1)	78(2)
C(10C)	7207(13)	-585(12)	3922(1)	76(2)
H	-322	3777	910	Uiso
C	418(9)	4082(2)	720(18)	Uani
H	1352	4044	860	Uiso
C	25(9)	4298(2)	640(18)	Uani
C	1099(4)	4439(1)	669(9)	Uani
H	1960(40)	4346(7)	570(100)	Uiso
H	1200(40)	4555(7)	590(100)	Uiso
C	1050(3)	4440(1)	552(7)	Uani
H	183	4355	660	Uiso
C	1074(5)	4594(1)	783(12)	Uani
H	1152	4513	1170	Uiso

H	1864	4689	1170	Uiso
H	222	4677	1170	Uiso
C	2285(2)	4282(1)	537(7)	Uani
C	3637(2)	4349(1)	613(8)	Uani
H	3796	4492	740	Uiso
C	4750(2)	4204(1)	738(11)	Uani
H	5654	4250	890	Uiso
C	4512(3)	3992(1)	825(12)	Uani
H	5257	3895	990	Uiso
C	3160(3)	3924(1)	836(12)	Uani
H	3001	3782	1000	Uiso
C	2047(2)	4069(1)	710(10)	Uani
H	1143	4024	850	Uiso
O	7329(9)	4874(1)	1010(20)	Uani
O	7765(7)	5189(1)	936(18)	Uani
O	4613(7)	4920(2)	1090(17)	Uani
H	4509	4802	1640	Uiso
O	5681(9)	4776(1)	1200(20)	Uani
H	5239	4694	1800	Uiso
O	2892(8)	4901(1)	1030(20)	Uani
O	3719(8)	5230(1)	980(20)	Uani
C	6975(7)	5046(1)	792(13)	Uani
C	5442(6)	5058(1)	751(10)	Uani
H	5110	5208	900	Uiso
C	5227(6)	4977(1)	723(10)	Uani
H	5865	5065	870	Uiso
C	3776(7)	5036(1)	721(14)	Uani
O	7088(11)	4803(1)	930(20)	Uani
O	8004(9)	5122(2)	940(20)	Uani
O	6420(8)	5122(2)	907(17)	Uani
H	5709	5154	1360	Uiso
O	4668(7)	5211(1)	987(19)	Uani
H	4695	5317	1480	Uiso
O	3185(9)	4819(1)	1040(20)	Uani
O	3026(9)	5176(1)	893(19)	Uani
C	7161(8)	4973(2)	822(15)	Uani
C	6066(7)	4972(1)	753(11)	Uani
H	6008	4826	900	Uiso

C	4652(7)	5033(1)	724(11)	Uani
H	4451	4918	870	Uiso

Computational studies:

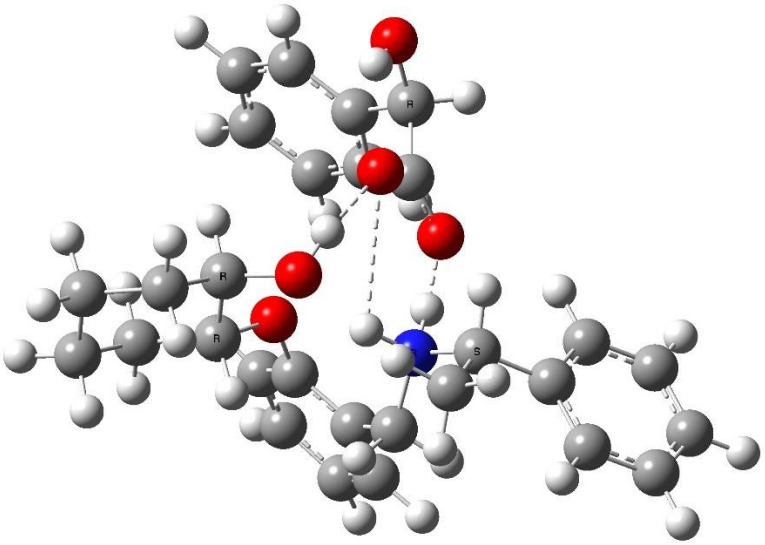


Figure 72: Optimized structure of diastereomeric complex (*R*,*R*,*S*)-**4** • (*R*)-**7**

C	2.71484	2.80727	-0.85637
C	1.42758	2.32857	-0.17893
C	1.56972	2.30332	1.3481
C	1.98752	3.67971	1.87404
C	3.26761	4.19032	1.19618
C	3.12686	4.1928	-0.33319
H	0.60067	3.00904	-0.4409
H	3.50595	2.07587	-0.64608
H	2.57799	2.82768	-1.94279
H	1.16131	4.38145	1.69483
H	2.11221	3.61531	2.95981
H	3.50884	5.19572	1.55924
H	4.11151	3.54642	1.47942
H	2.37142	4.93451	-0.62844
H	4.06577	4.50282	-0.80529
H	2.34547	1.56264	1.5882
O	0.34328	1.90911	1.96327
H	0.42252	0.95459	2.24198
O	1.06909	0.98118	-0.55346
C	0.55797	0.75262	-1.81381

C	1.41872	0.30865	-2.82096
C	-0.82546	0.85416	-2.05231
C	0.92281	0.00069	-4.08642
H	2.46911	0.18552	-2.5822
C	-1.30256	0.53058	-3.32891
C	-0.44232	0.1199	-4.34575
H	1.60069	-0.34229	-4.86222
H	-2.37032	0.59409	-3.52293
H	-0.84009	-0.12599	-5.32528
C	-1.81943	1.31205	-1.00409
H	-1.79273	2.40105	-0.88339
H	-2.82623	1.04579	-1.33125
N	-1.60621	0.70836	0.34503
H	-1.18974	-0.30338	0.32573
C	-2.79791	0.70224	1.28364
H	-2.41308	0.14225	2.14316
C	-3.96007	-0.08304	0.68728
C	-3.80372	-1.45986	0.45398
C	-5.1881	0.51559	0.37946
C	-4.84976	-2.21049	-0.07885
H	-2.85417	-1.938	0.67984
C	-6.23747	-0.23979	-0.15001
H	-5.34165	1.5743	0.55974
C	-6.07114	-1.60393	-0.38137
H	-4.71145	-3.27348	-0.2527
H	-7.18393	0.24179	-0.37786
H	-6.887	-2.19199	-0.79129
C	-3.11046	2.1255	1.74643
H	-3.888	2.10541	2.5144
H	-2.21266	2.57665	2.17679
H	-3.4622	2.76494	0.93093
C	0.28272	-1.61478	1.6136
C	1.1733	-2.86208	1.83854
H	0.51908	-3.74117	1.75423
C	2.24554	-2.94932	0.74848
C	3.59808	-2.84814	1.08559
C	1.89143	-3.13801	-0.59451
C	4.58271	-2.93011	0.09854
H	3.86117	-2.71989	2.12945
C	2.87516	-3.21903	-1.57943
H	0.84169	-3.20022	-0.86178
C	4.2261	-3.11515	-1.23735
H	5.63085	-2.85415	0.37638
H	2.58574	-3.36638	-2.61666
H	4.99233	-3.18469	-2.00485
O	1.72776	-2.81821	3.13464
H	1.54507	-1.9037	3.42386

O	0.43551	-0.68086	2.45108
O	-0.51611	-1.63969	0.63202
H	-0.85067	1.23527	0.83289

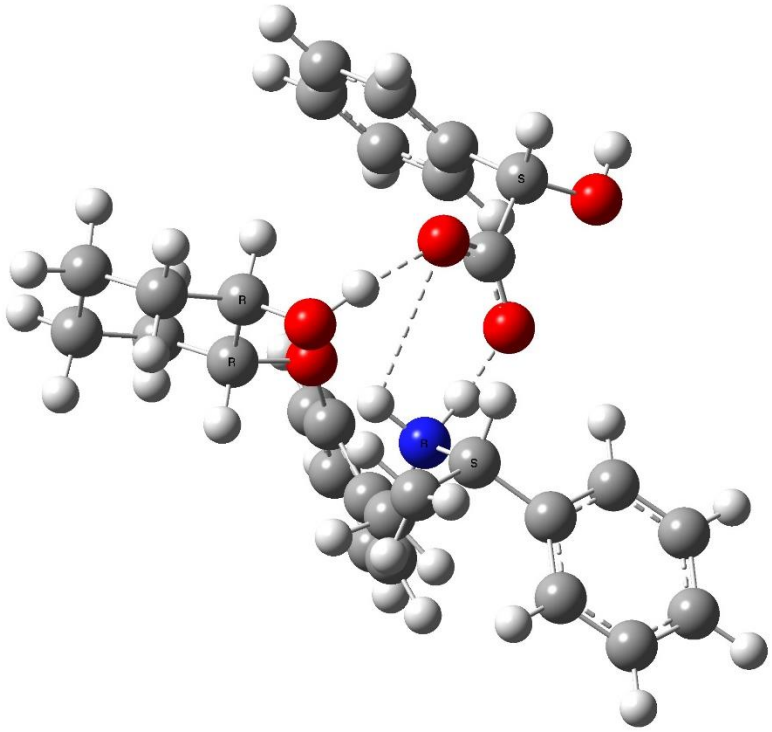


Figure 73: Optimized structure of diastereomeric complex (*R*,*R*,*S*)-**4** • (*S*)-**7**

C	3.08271	-2.39741	0.65007
C	1.81319	-1.98617	-0.10109
C	2.12195	-1.60894	-1.55797
C	2.81293	-2.77981	-2.26577
C	4.07682	-3.24017	-1.52586
C	3.77535	-3.57414	-0.0574
H	1.10203	-2.82783	-0.10352
H	3.75767	-1.53227	0.68958
H	2.83829	-2.66244	1.68391
H	2.09563	-3.60902	-2.33916
H	3.04333	-2.47568	-3.29189
H	4.51518	-4.10784	-2.0322
H	4.83175	-2.44273	-1.56446
H	3.12627	-4.45975	-0.01142
H	4.69689	-3.83787	0.47399
H	2.80783	-0.74797	-1.52779

O	0.9497	-1.27039	-2.27581
H	0.79452	-0.30817	-2.16554
O	1.16797	-0.83051	0.48336
C	0.52316	-0.98248	1.6882
C	1.19649	-0.70145	2.87982
C	-0.8439	-1.31878	1.70915
C	0.52668	-0.78526	4.10016
H	2.23468	-0.39369	2.82543
C	-1.49922	-1.3913	2.94363
C	-0.82194	-1.13891	4.1362
H	1.05774	-0.56368	5.02121
H	-2.55669	-1.64223	2.96704
H	-1.34908	-1.20117	5.08291
C	-1.60953	-1.56886	0.43203
H	-1.16196	-2.36344	-0.16775
H	-2.63741	-1.85183	0.67028
N	-1.66884	-0.35473	-0.43982
H	-1.70777	0.54946	0.09675
C	-2.74787	-0.32086	-1.50084
H	-2.48538	0.58087	-2.06254
C	-4.11054	-0.10606	-0.8578
C	-4.35843	1.11978	-0.21708
C	-5.12448	-1.06997	-0.88562
C	-5.58875	1.36593	0.38795
H	-3.57825	1.87792	-0.1925
C	-6.36047	-0.81945	-0.28301
H	-4.96394	-2.01853	-1.38746
C	-6.59466	0.39642	0.35653
H	-5.76387	2.31853	0.879
H	-7.13842	-1.57661	-0.31838
H	-7.55566	0.59108	0.82355
C	-2.60284	-1.52138	-2.43446
H	-3.26576	-1.39913	-3.29494
H	-1.5722	-1.59037	-2.79385
H	-2.85879	-2.46726	-1.94808
C	-0.15554	2.1558	-0.91576
C	0.84943	3.32564	-1.03724
C	2.17229	2.90171	-0.41323
C	3.20654	2.37449	-1.19444
C	2.35475	3.01613	0.9708
C	4.40538	1.9689	-0.60564
H	3.07026	2.28725	-2.26919
C	3.55407	2.61476	1.56006

H	1.54659	3.42345	1.56984
C	4.58269	2.08838	0.7748
H	5.20502	1.57185	-1.22514
H	3.68784	2.71623	2.63388
H	5.51954	1.7839	1.23323
O	0.03523	1.20292	-1.73898
O	-1.04272	2.20585	-0.03091
H	-0.77325	-0.1568	-0.94866
O	0.30316	4.47667	-0.41298
H	0.99258	5.15449	-0.42766
H	1.00215	3.48865	-2.11431

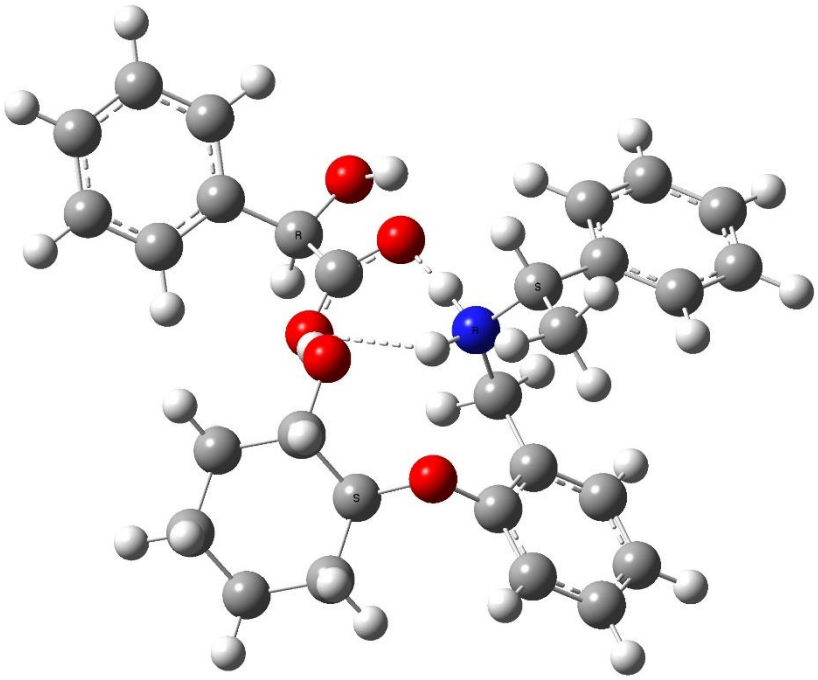


Figure 74: Optimized structure of diastereomeric complex (*S*,*S*,*S*)-**4** • (*R*)-**7**

C	-2.70394	-2.09923	-0.865
C	-2.06938	-0.87033	-0.1597
C	-3.04813	0.31346	-0.25334
C	-4.35904	-0.05498	0.46862
C	-4.98576	-1.29578	-0.19292
C	-3.99724	-2.47584	-0.12029
H	-2.61561	1.17276	0.21419
H	-1.88283	-1.09458	0.86987
H	-2.93915	-1.86985	-1.88353
H	-4.1491	-0.26906	1.4959

H	-5.04345	0.76517	0.40726
H	-5.88891	-1.55378	0.31888
H	-5.20531	-1.08047	-1.21807
H	-3.77142	-2.69535	0.90238
H	-4.43709	-3.33592	-0.58032
H	-3.25003	0.53103	-1.28144
O	-1.7805	-3.18209	-0.83708
H	-1.39276	-3.143	0.01266
O	-0.83285	-0.53851	-0.78617
C	-0.34583	0.74223	-0.34915
C	0.60471	0.9464	0.70202
C	-0.8438	1.85476	-1.04696
C	1.07944	2.24891	0.93591
C	-0.38202	3.14348	-0.77019
H	-1.58446	1.71191	-1.80545
C	0.59086	3.33822	0.20835
H	1.82423	2.40974	1.68706
H	-0.77271	3.97973	-1.31107
H	0.96264	4.32202	0.40392
C	1.19577	-0.152	1.63564
H	0.7016	-0.12483	2.58451
H	2.2371	0.05907	1.76113
N	1.02917	-1.4968	1.08718
H	1.39459	-2.20761	1.58378
C	1.56047	-1.47346	-0.28466
H	1.44854	-2.44169	-0.72643
C	3.05221	-1.09489	-0.25387
C	4.02659	-2.0964	-0.14718
C	3.43517	0.25012	-0.33337
C	5.38451	-1.75233	-0.11946
H	3.73358	-3.12392	-0.08755
C	4.79301	0.59438	-0.30572
H	2.69061	1.01454	-0.41568
C	5.76777	-0.40669	-0.19781
H	6.12883	-2.51699	-0.0382
H	5.08543	1.62182	-0.36681
H	6.80482	-0.14376	-0.17525
C	0.78572	-0.43685	-1.11847
H	-0.25063	-0.70126	-1.1429
H	0.89677	0.53131	-0.67633
H	1.17303	-0.41992	-2.11591
H	0.14955	-1.84544	1.14537
C	-0.35681	-5.41794	1.72624

H	-1.39945	-5.45198	1.96498
C	-0.11325	-6.10754	0.37097
C	-0.94136	-7.15727	-0.04822
C	0.94286	-5.67935	-0.44527
C	-0.71429	-7.77644	-1.28551
H	-1.74652	-7.48618	0.57486
C	1.16994	-6.29814	-1.68143
H	1.57599	-4.87896	-0.12411
C	0.34109	-7.34639	-2.10202
H	-1.3463	-8.57737	-1.60688
H	1.97631	-5.97013	-2.30405
H	0.51438	-7.81856	-3.04657
O	0.38618	-6.08924	2.74687
H	0.23586	-5.65554	3.58997
C	0.10374	-3.9525	1.63202
O	-0.73978	-2.94821	1.25267
O	1.37413	-3.57304	1.93092

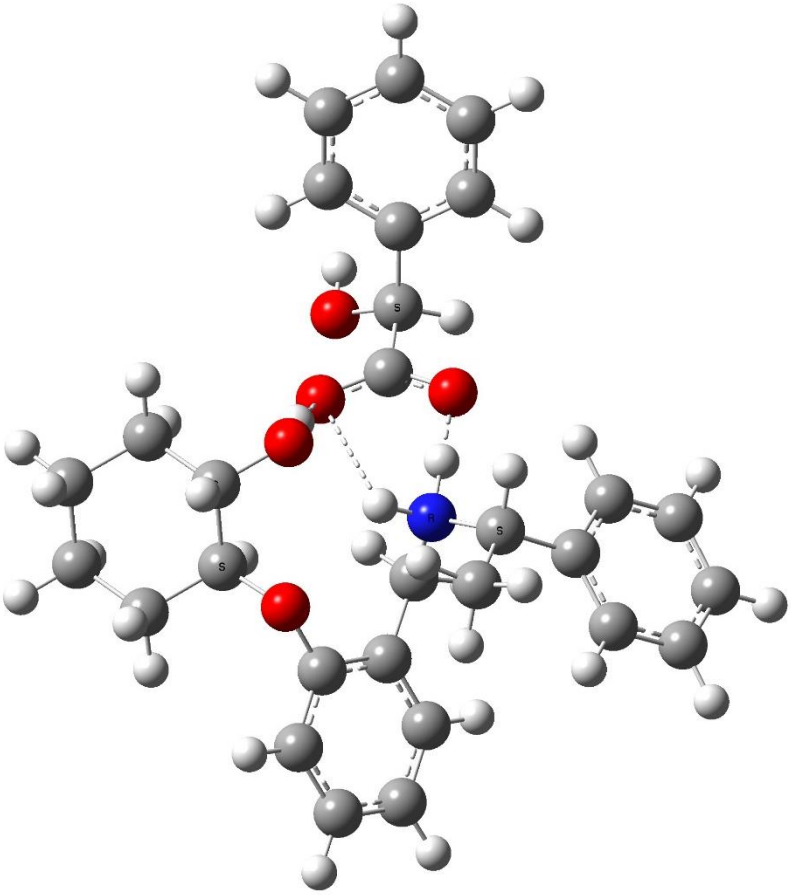


Figure 75: Optimized structure of diastereomeric complex (*S*,*S*,*S*)-**4** • (*S*)-**7**

C	-0.21258	-2.95029	-1.12273
C	-1.40259	-2.80459	-0.16386
C	-2.10319	-4.14328	0.08118
C	-1.11268	-5.19123	0.61421
C	0.08256	-5.35597	-0.33602
C	0.77131	-4.00976	-0.60468
H	-2.93601	-4.00584	0.77969
H	-1.03951	-2.39669	0.78996
H	-0.62073	-3.27153	-2.09141
H	-0.75065	-4.88082	1.6039
H	-1.62697	-6.14842	0.75701
H	0.80355	-6.06928	0.07907
H	-0.26835	-5.78442	-1.2854
H	1.233	-3.63182	0.3172
H	1.5781	-4.11878	-1.3372
H	-2.53366	-4.48532	-0.8696
O	0.42511	-1.70565	-1.35916
H	0.97356	-1.47148	-0.56032
O	-2.29058	-1.83894	-0.78686
C	-3.21734	-1.19251	0.00195
C	-2.86559	-0.01405	0.68926
C	-4.53669	-1.65236	0.01191
C	-3.86904	0.66224	1.39478
C	-5.51787	-0.96483	0.72603
H	-4.77593	-2.54424	-0.55734
C	-5.18313	0.1947	1.42428
H	-3.61184	1.57655	1.92276
H	-6.53966	-1.33252	0.73006
H	-5.93978	0.7397	1.97997
C	-1.44851	0.51162	0.73728
H	-0.78846	-0.174	1.27872
H	-1.42922	1.46226	1.27217
N	-0.73927	0.72992	-0.56299
H	0.30449	0.97502	-0.25704
C	-1.23251	1.78304	-1.53005
H	-0.36547	1.92824	-2.18587
C	-1.48597	3.10751	-0.81668
C	-0.40733	3.77717	-0.21423
C	-2.75662	3.69203	-0.75779
C	-0.60285	4.99656	0.43203
H	0.58314	3.33068	-0.23037

C	-2.94928	4.91756	-0.11526
H	-3.60637	3.19943	-1.21714
C	-1.87395	5.57326	0.48147
H	0.24172	5.49891	0.89447
H	-3.9421	5.35703	-0.08485
H	-2.02318	6.52645	0.98023
C	-2.37964	1.25853	-2.39464
H	-2.09213	0.31544	-2.86646
H	-3.28984	1.08025	-1.81962
H	-2.60441	1.98118	-3.1842
H	-0.63307	-0.18241	-1.05138
C	3.46542	0.55031	1.61919
C	4.62006	0.53664	0.62638
C	5.295	-0.65965	0.35482
C	5.00201	1.70298	-0.04644
C	6.34427	-0.68433	-0.56459
H	4.98479	-1.5624	0.87101
C	6.0482	1.67737	-0.96822
H	4.4713	2.63003	0.15206
C	6.72484	0.48346	-1.22794
H	6.86285	-1.6177	-0.76614
H	6.33897	2.59024	-1.48076
H	7.54308	0.46431	-1.94223
C	2.14819	0.25882	0.86349
O	1.70584	-0.91146	0.84078
O	1.63396	1.27666	0.29139
H	3.36614	1.56353	2.03452
O	3.61909	-0.41405	2.64864
H	4.49309	-0.26942	3.03628