Supporting Information For:

Synthesis of enantiomerically pure helicene-like mono 1,3-oxazines from 1,1'-binaphthyl-2,2',7-triol and study of their chiroptical properties

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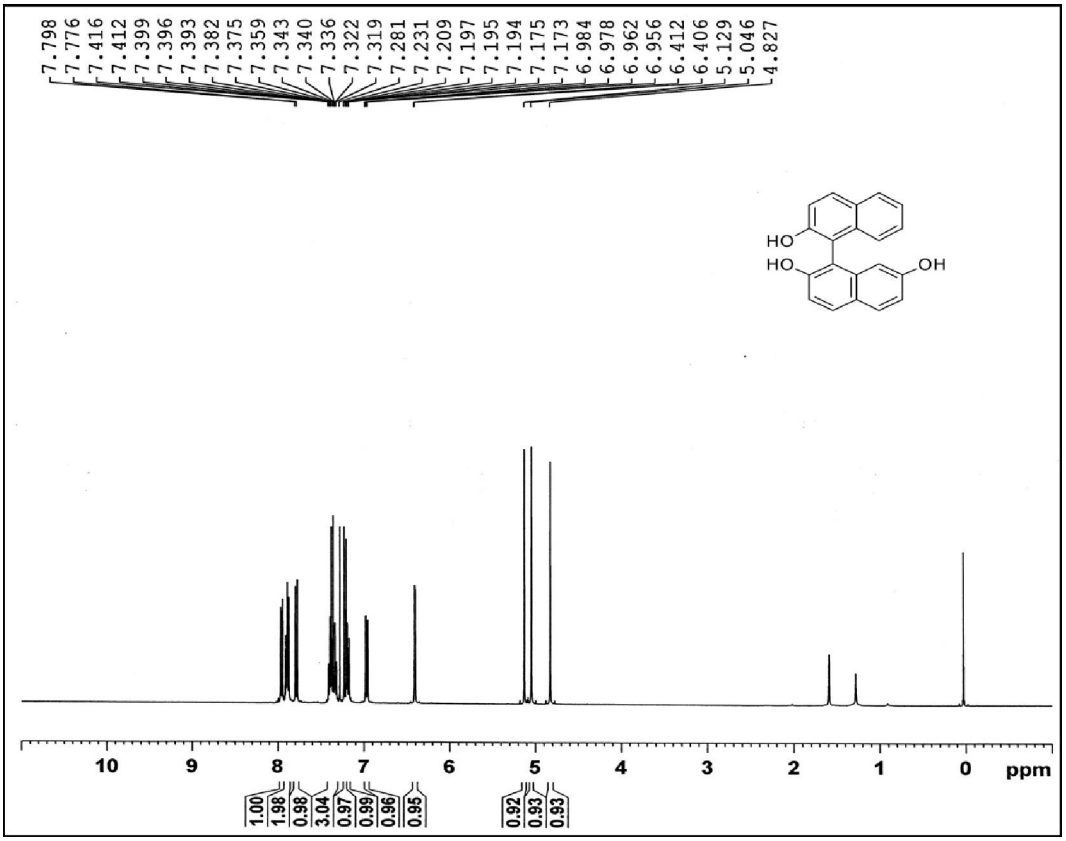
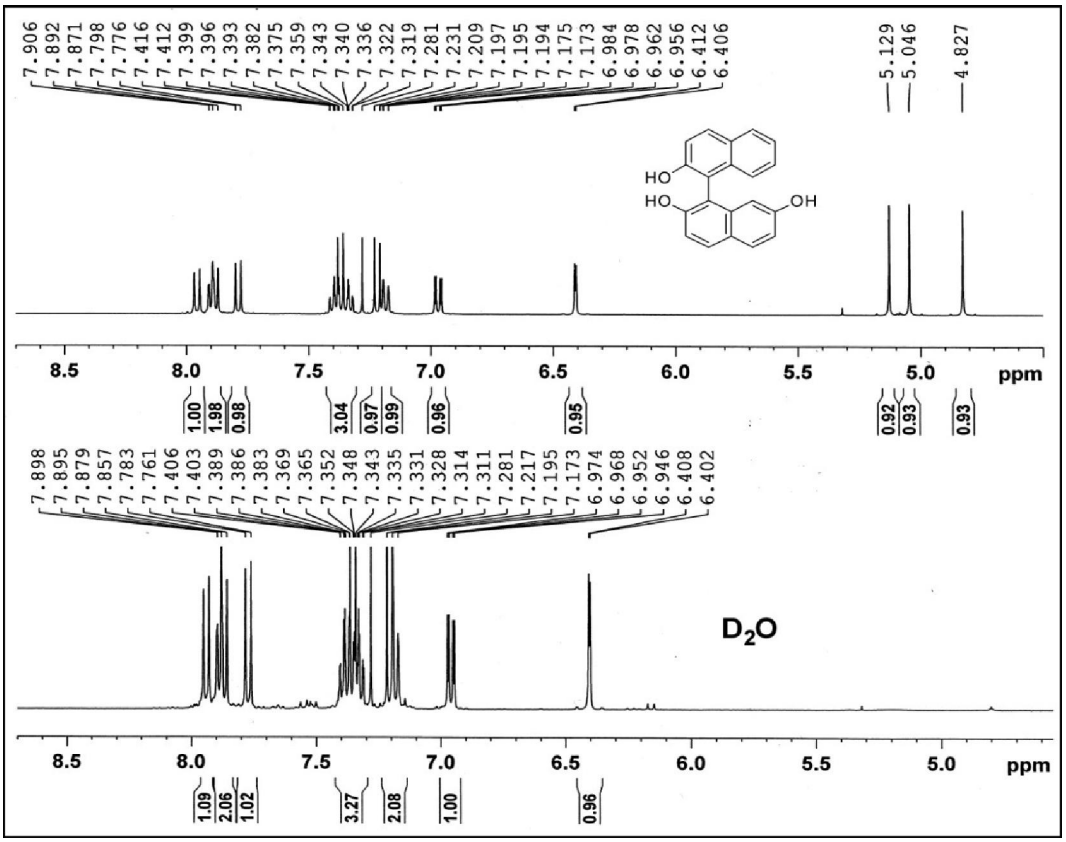
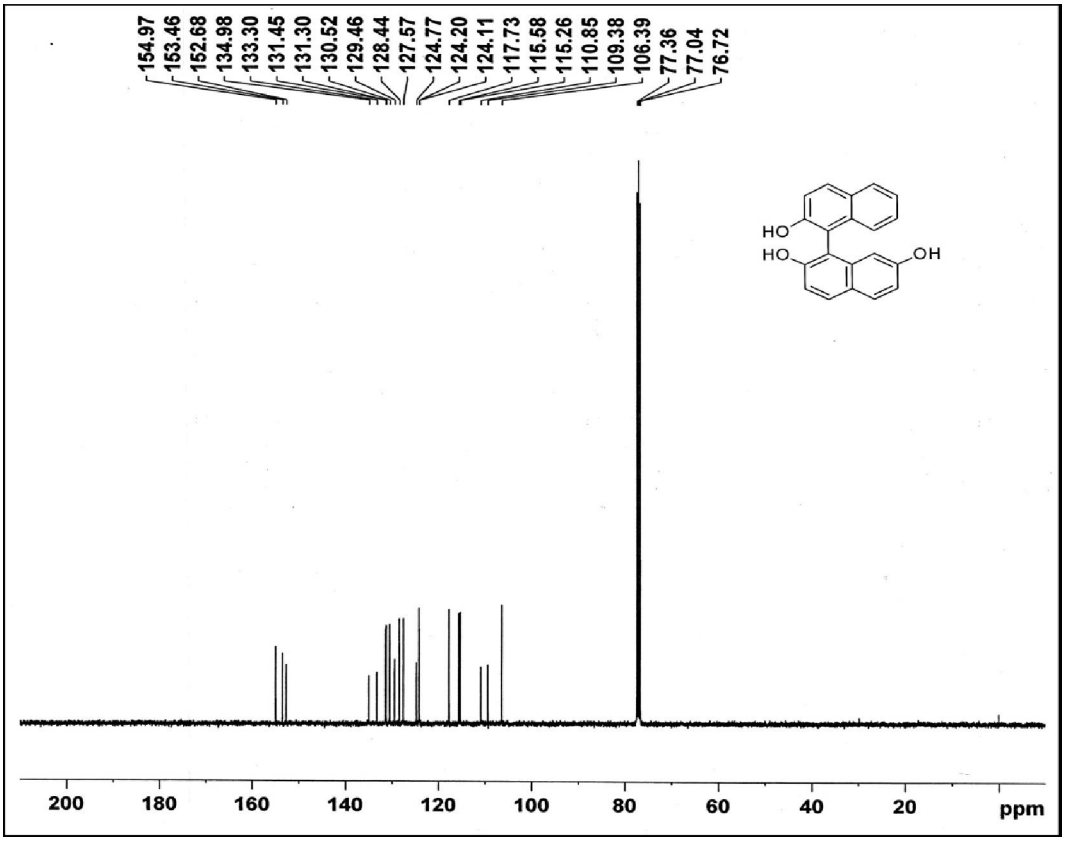
Contents:

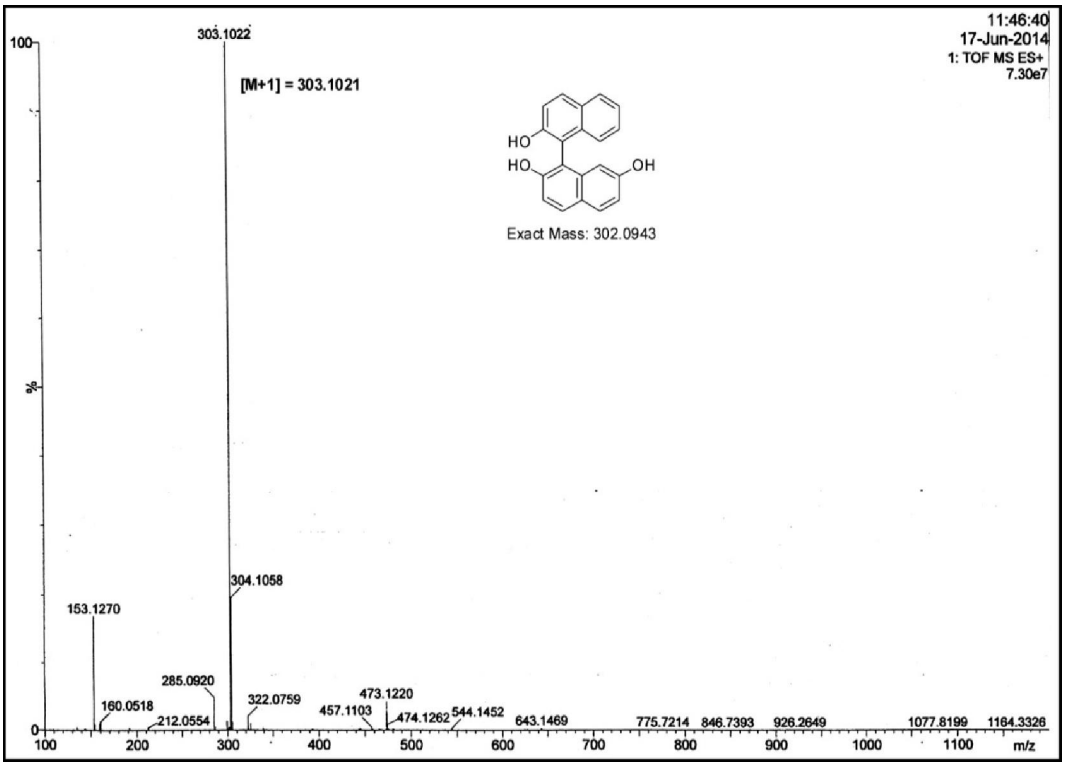


^{1}H-NMR Spectrum of compound 1





^{13}C-NMR spectrum of compound 1



HRMS spectrum of compound 1

HPLC analysis of compound 1:

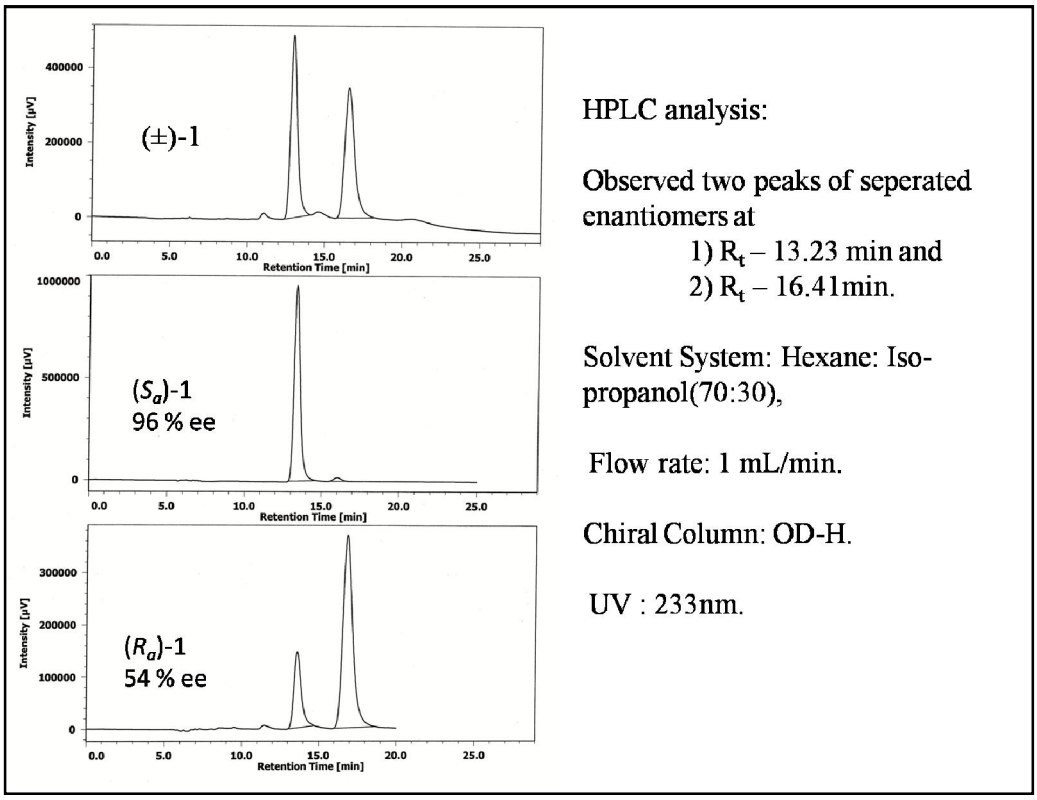
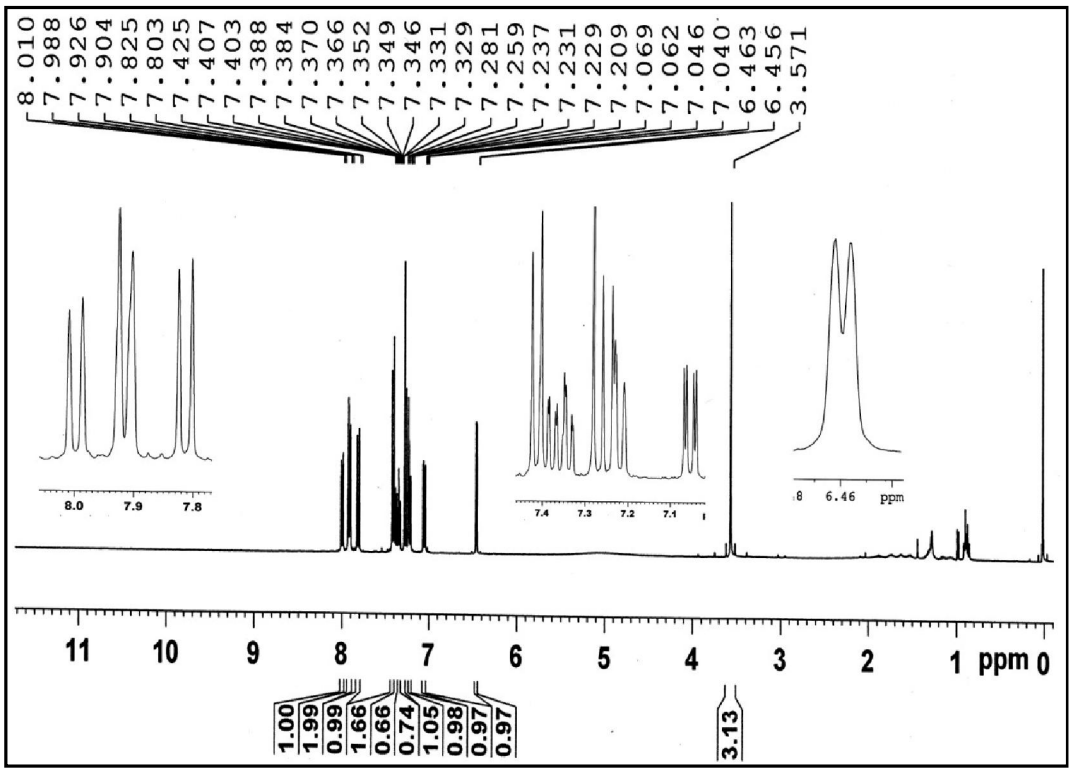
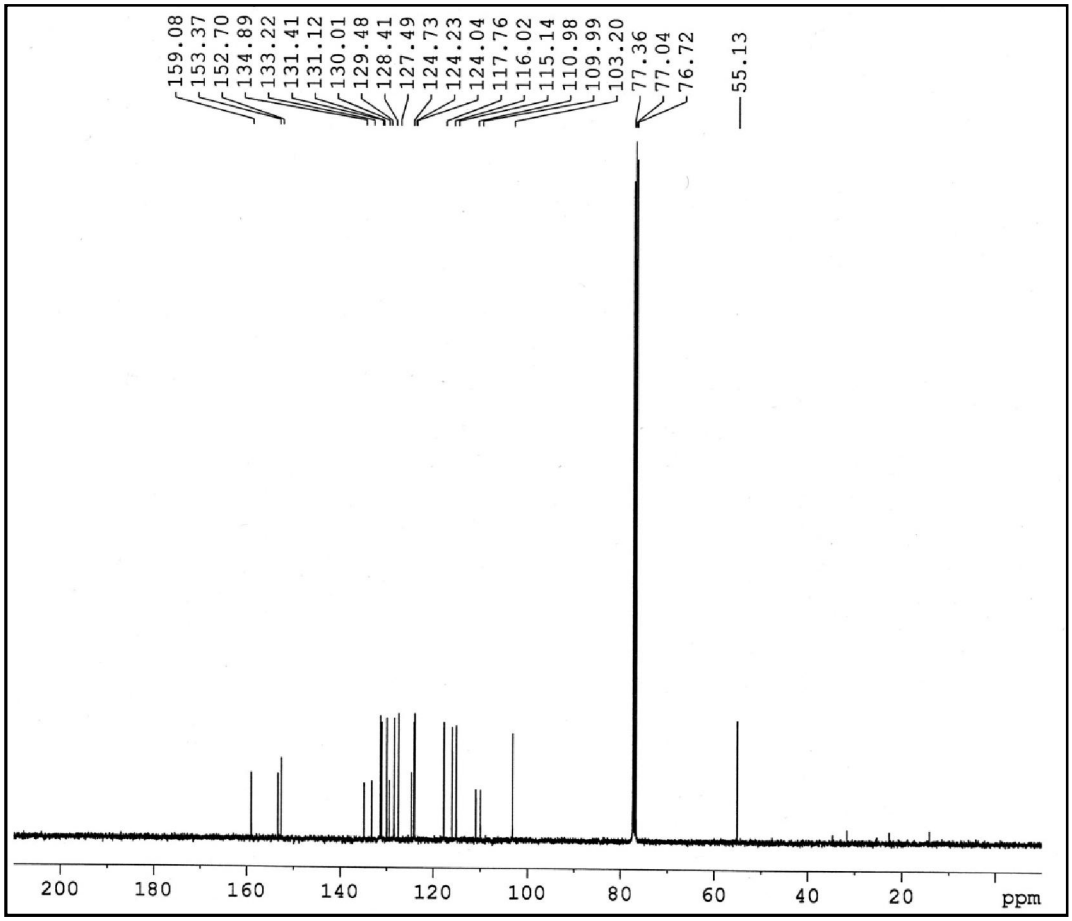


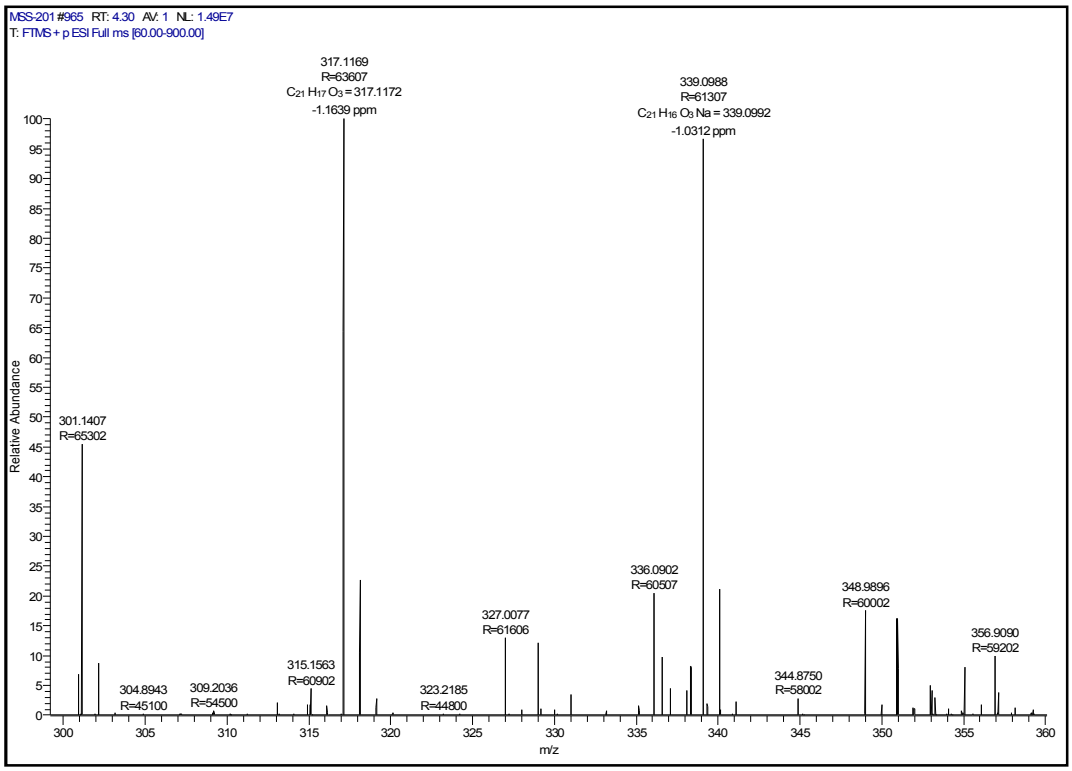
Figure 1: HPLC analysis of enantiomers pair of (S_a)-**1** and (R_a)-**1**



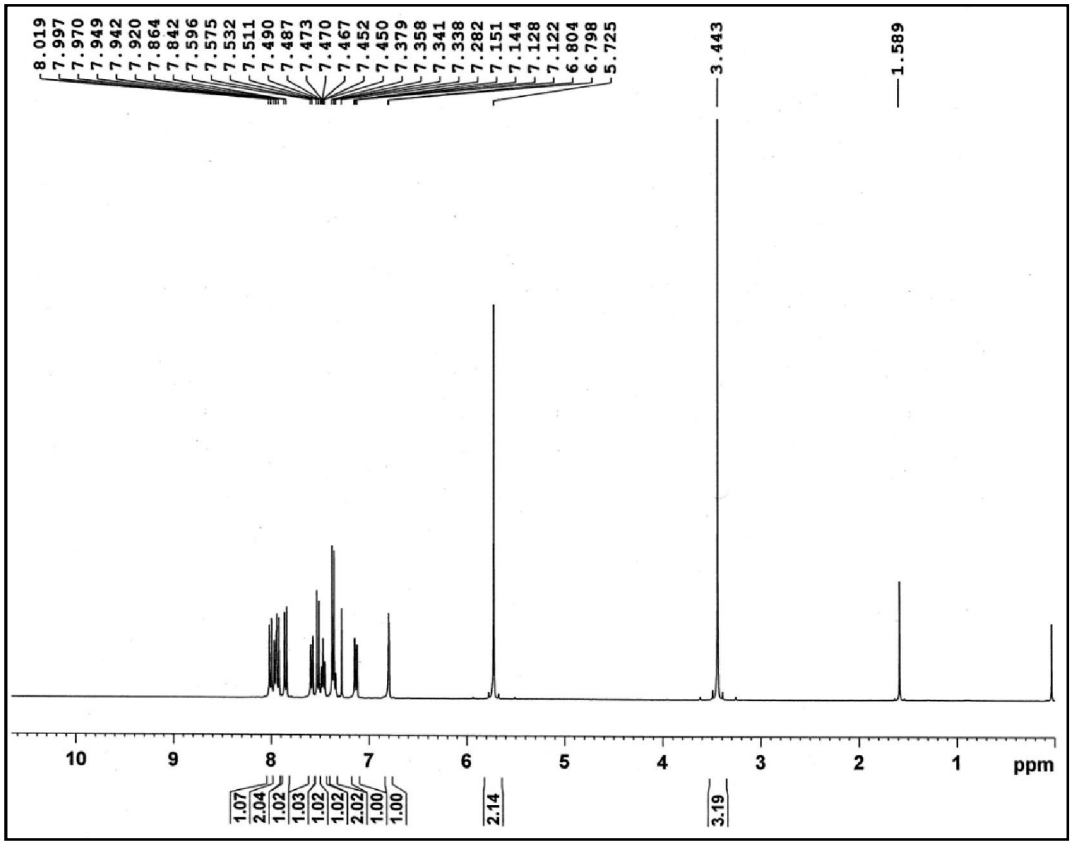
^{1}H-NMR Spectrum of compound (±)-8



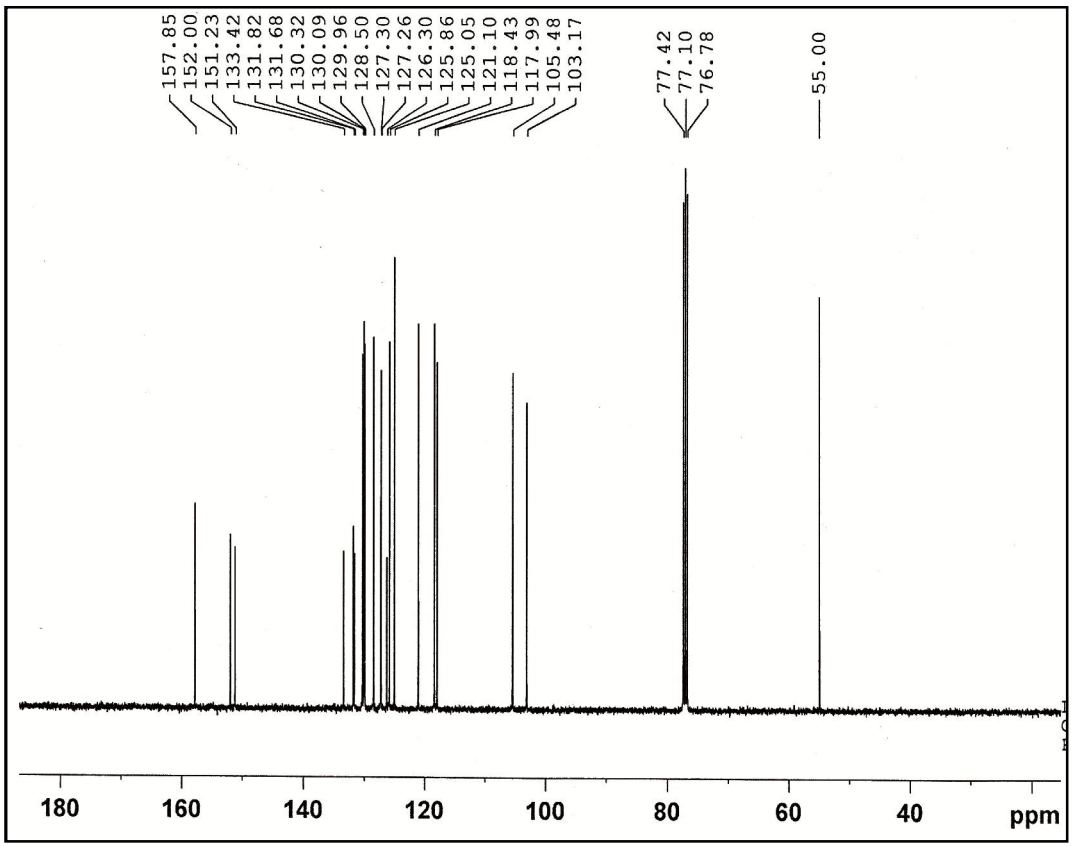
^{13}C-NMR spectrum of compound (±)-8



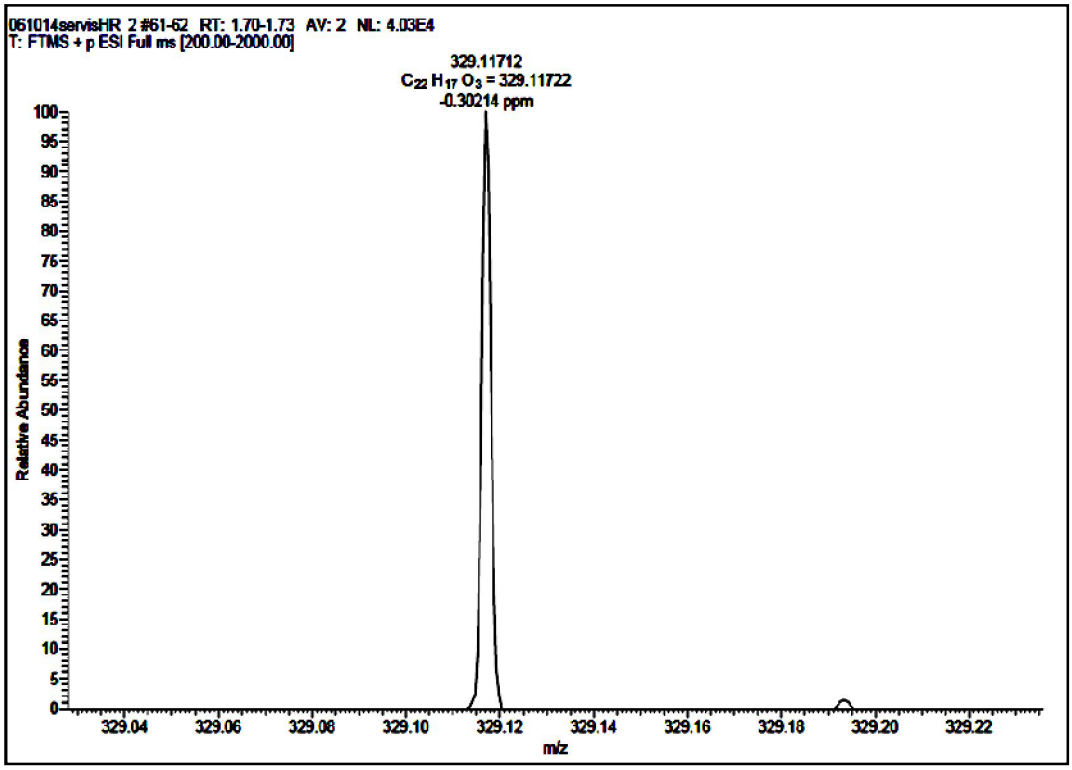
HRMS spectrum of compound (±)-8



^{1}H-NMR Spectrum of compound (±)-9



^{13}C-NMR spectrum of compound (±)-9



HRMS spectrum of compound (±)-9

HPLC analysis of compound 9:

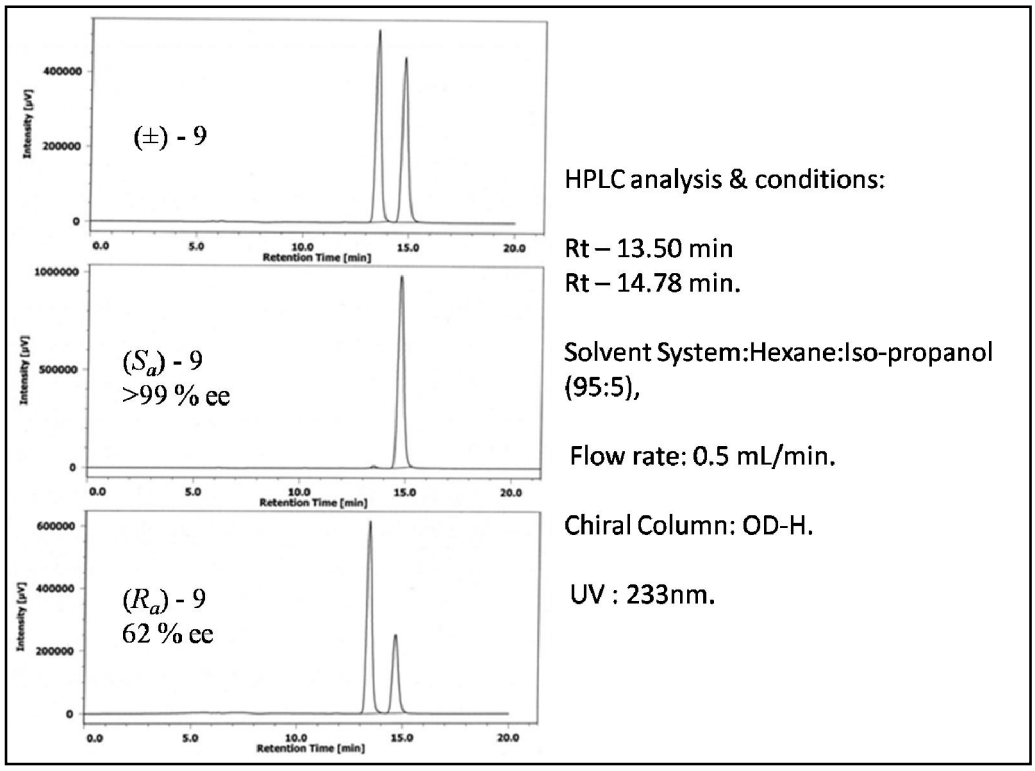
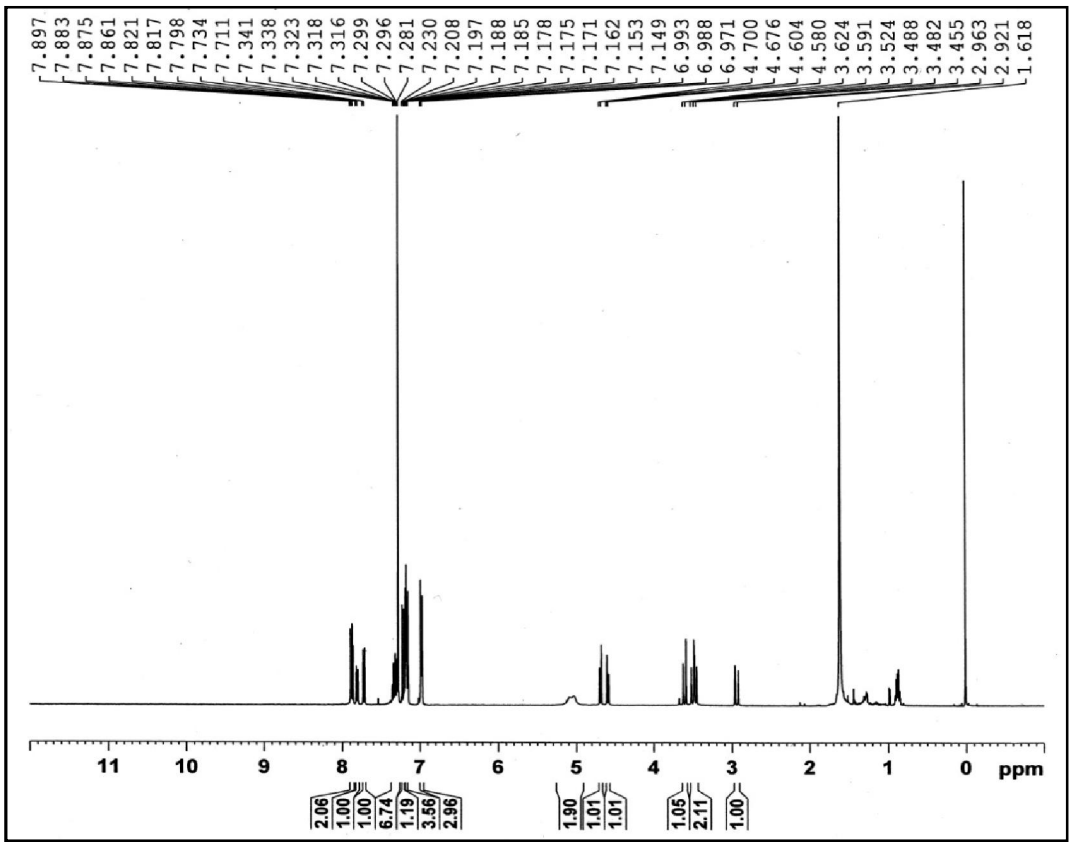
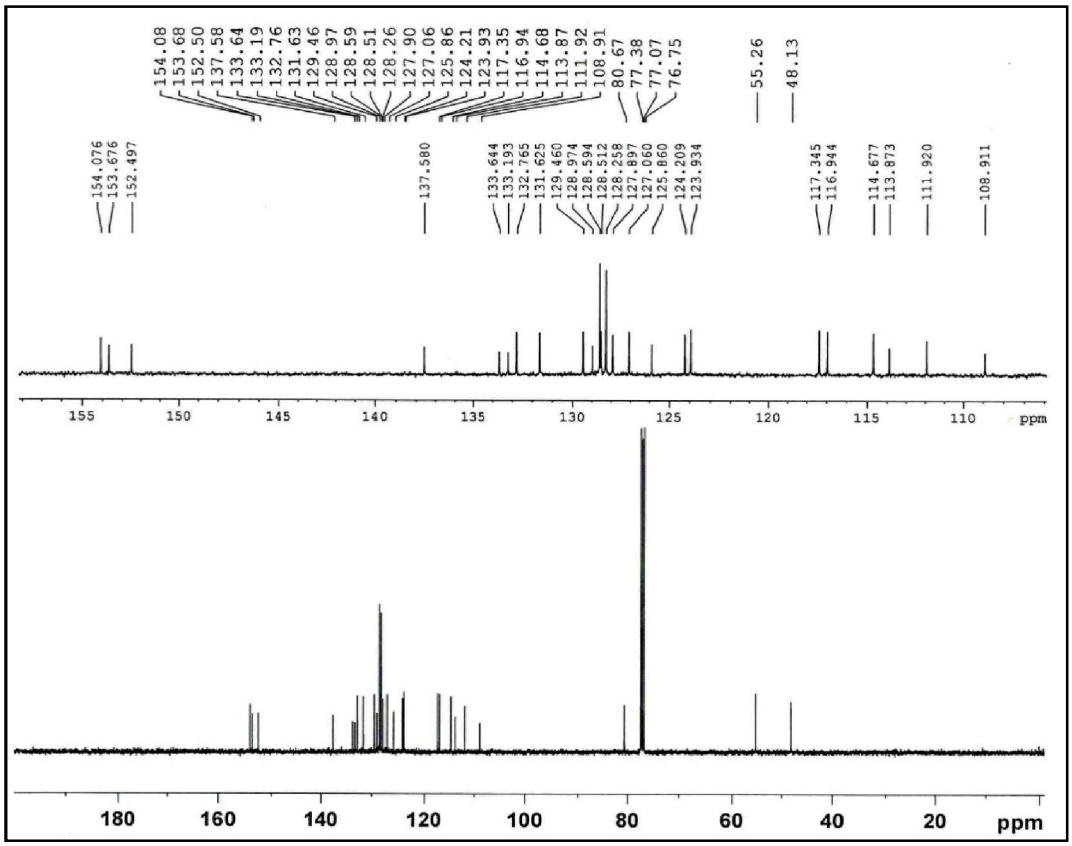


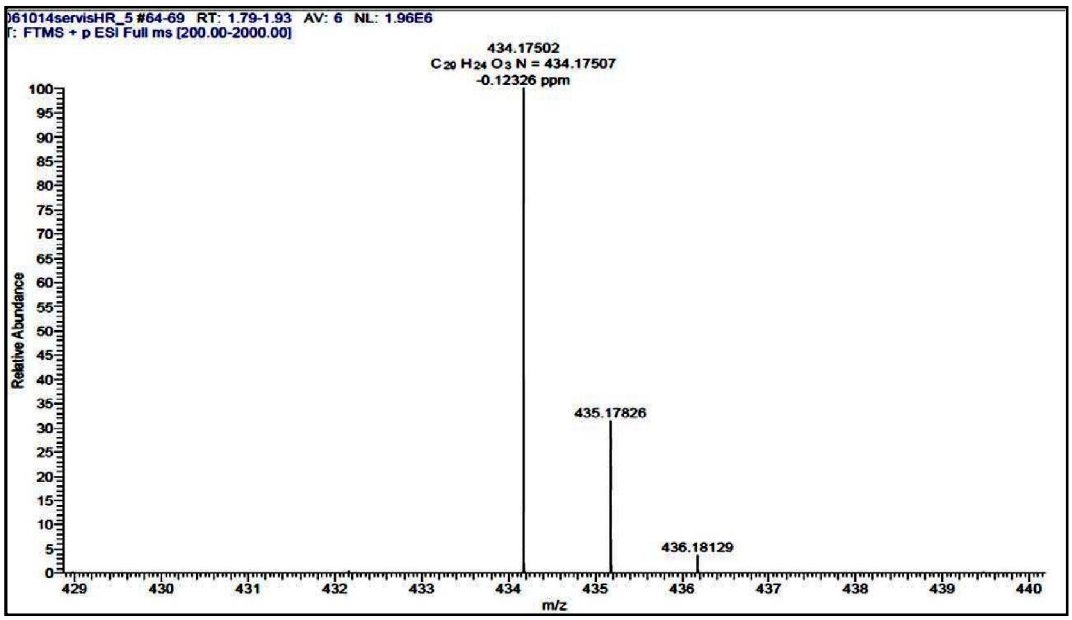
Figure 2: HPLC analysis of enantiomers pair of (*P*)-**9** and (*M*)-**9**



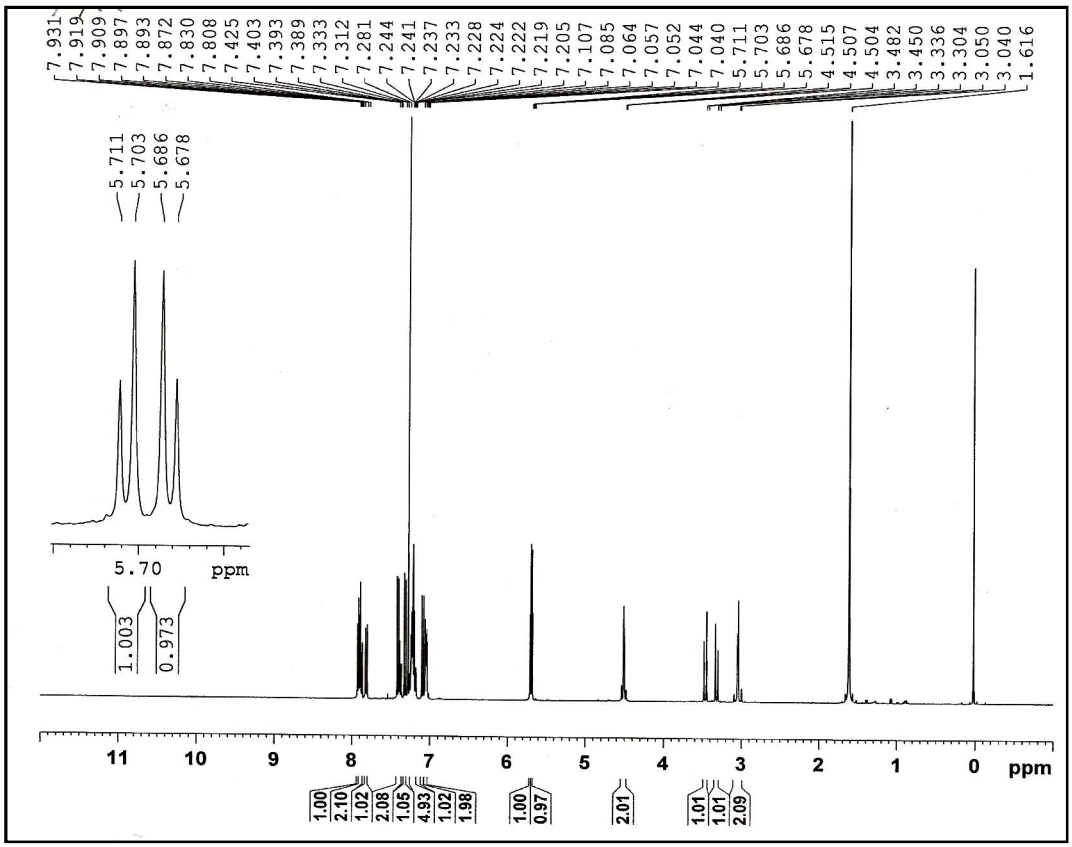
^{1}H-NMR Spectrum of compound (±)-10



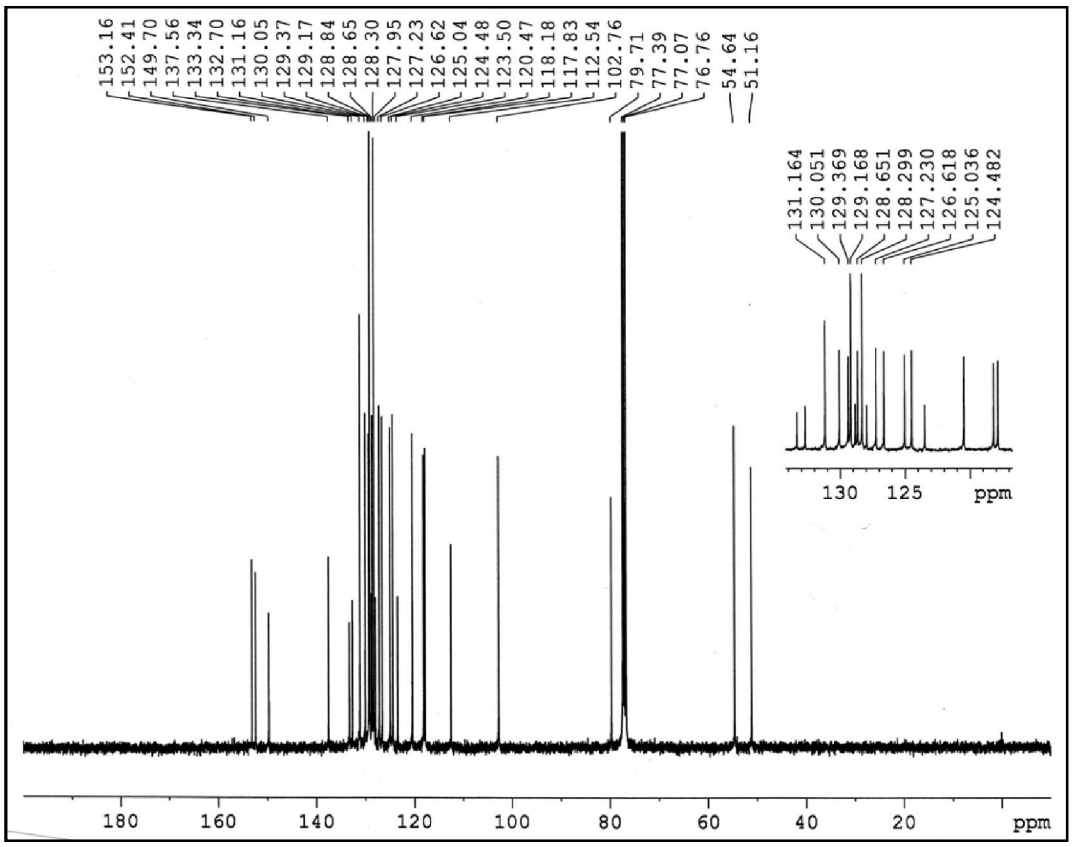
^{13}C-NMR spectrum of compound (±)-10



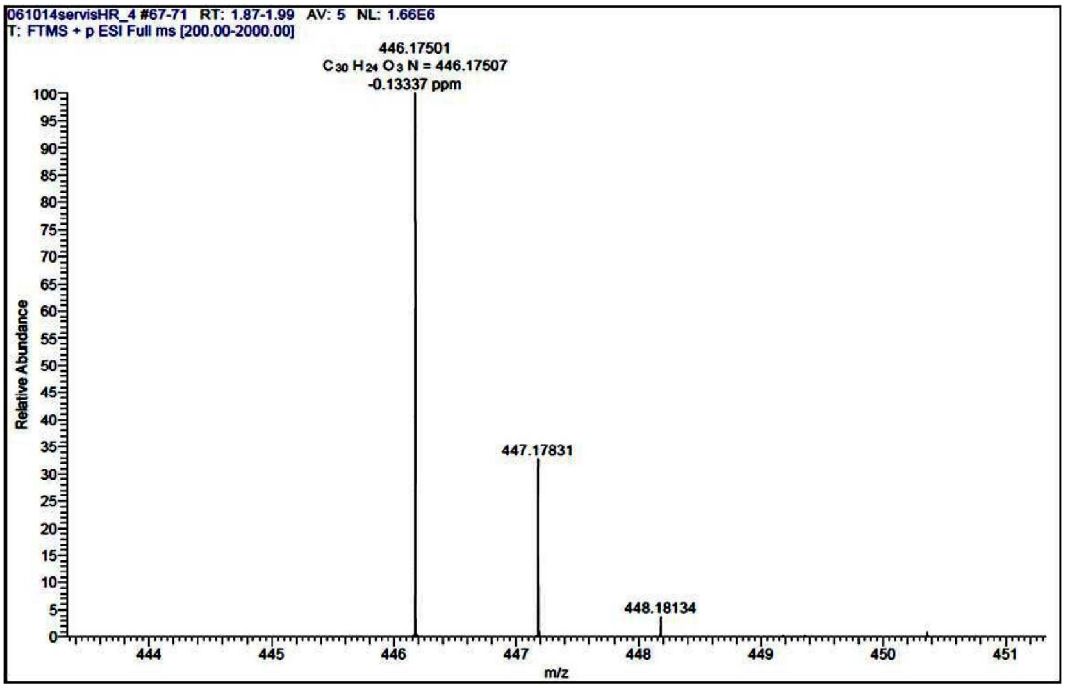
HRMS spectrum of compound (±)-10



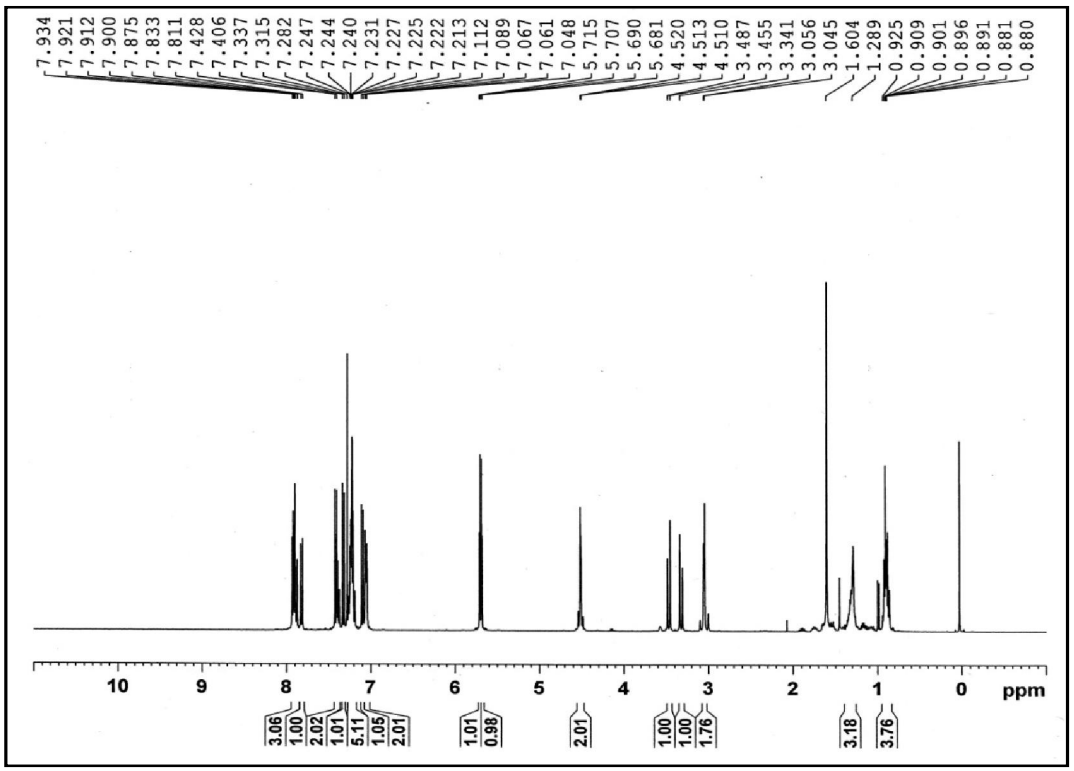
^{1}H-NMR Spectrum of compound (±)-11



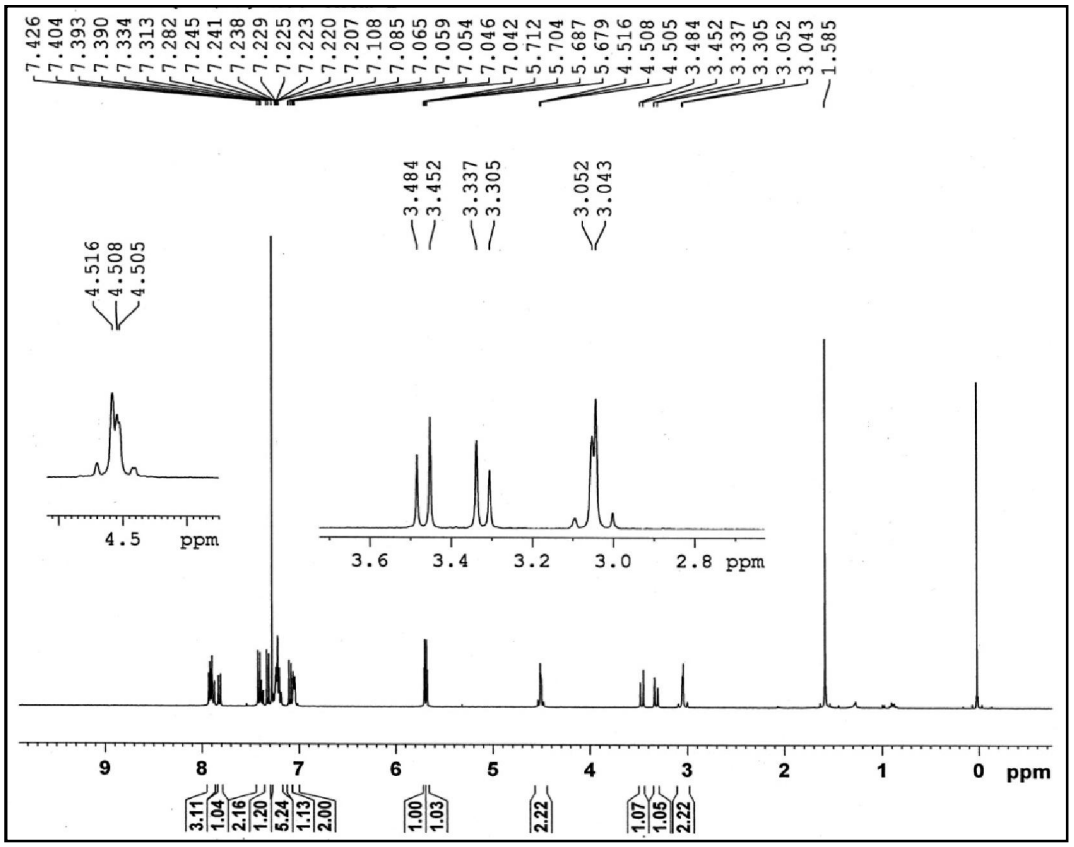
^{13}C-NMR spectrum of compound (±)-11



HRMS spectrum of compound (±)-11



^{1}H-NMR Spectrum of compound [(*P*)-11]



^{1}H-NMR Spectrum of compound [(*M*)-11]

HPLC Analysis of compound 11:

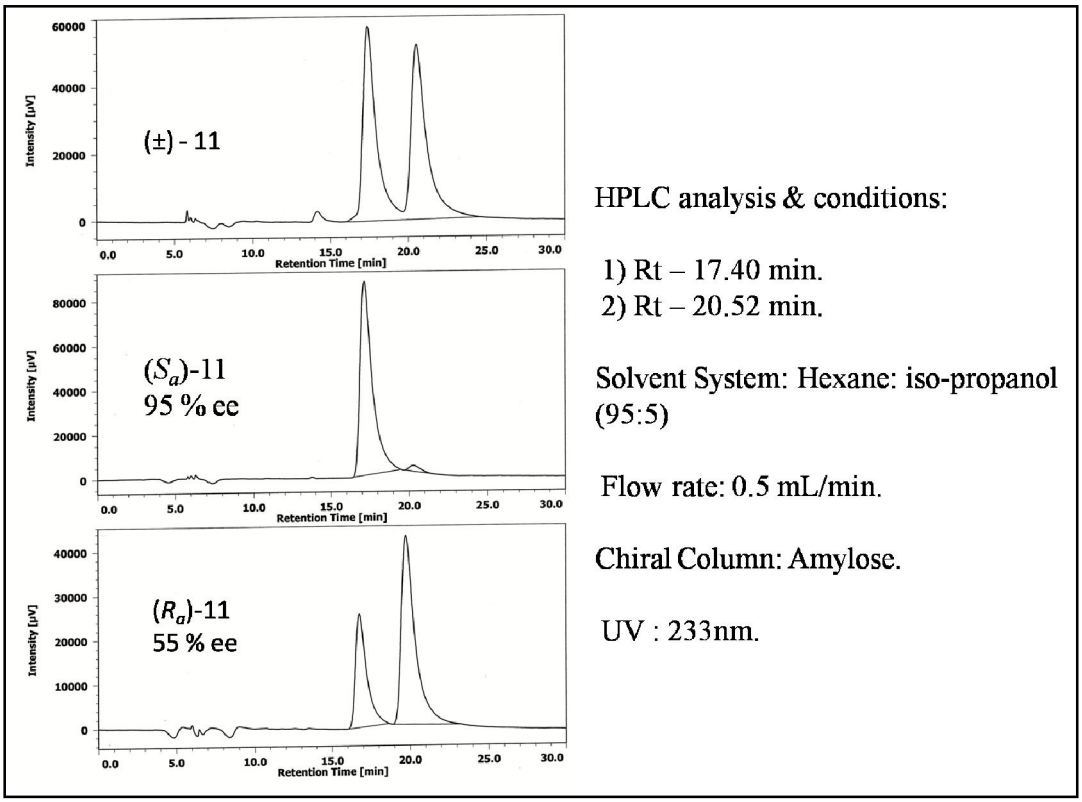
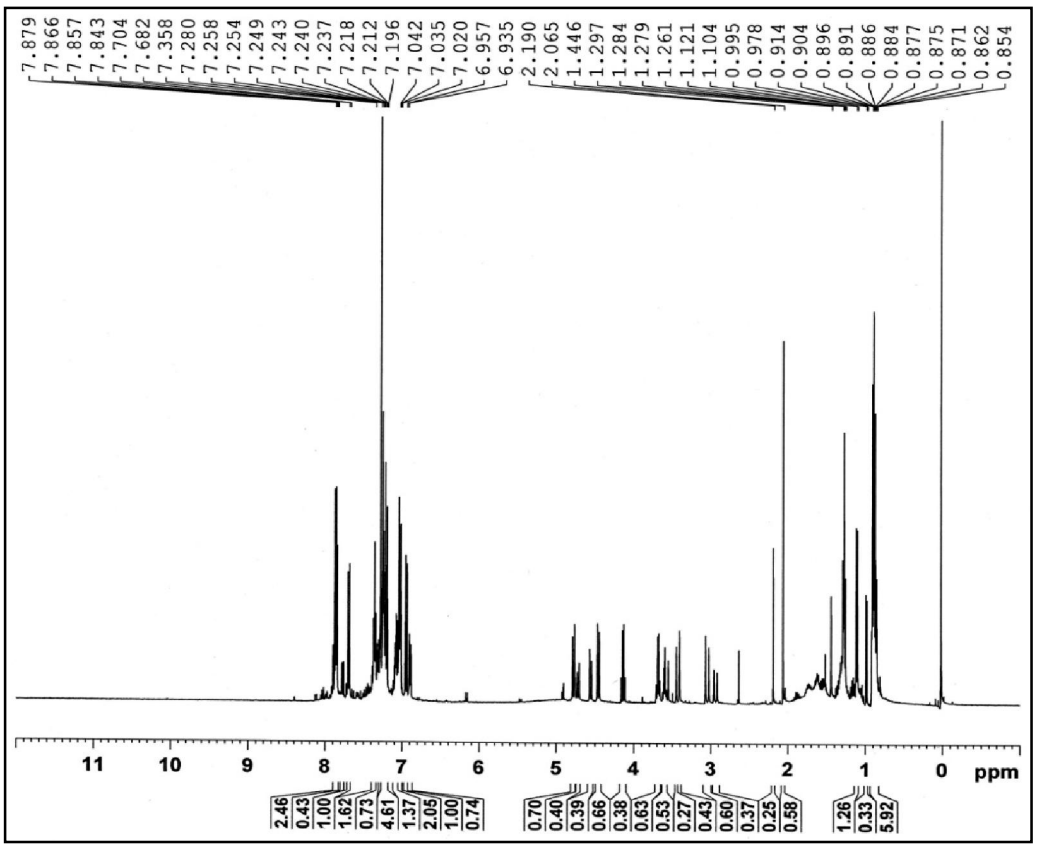
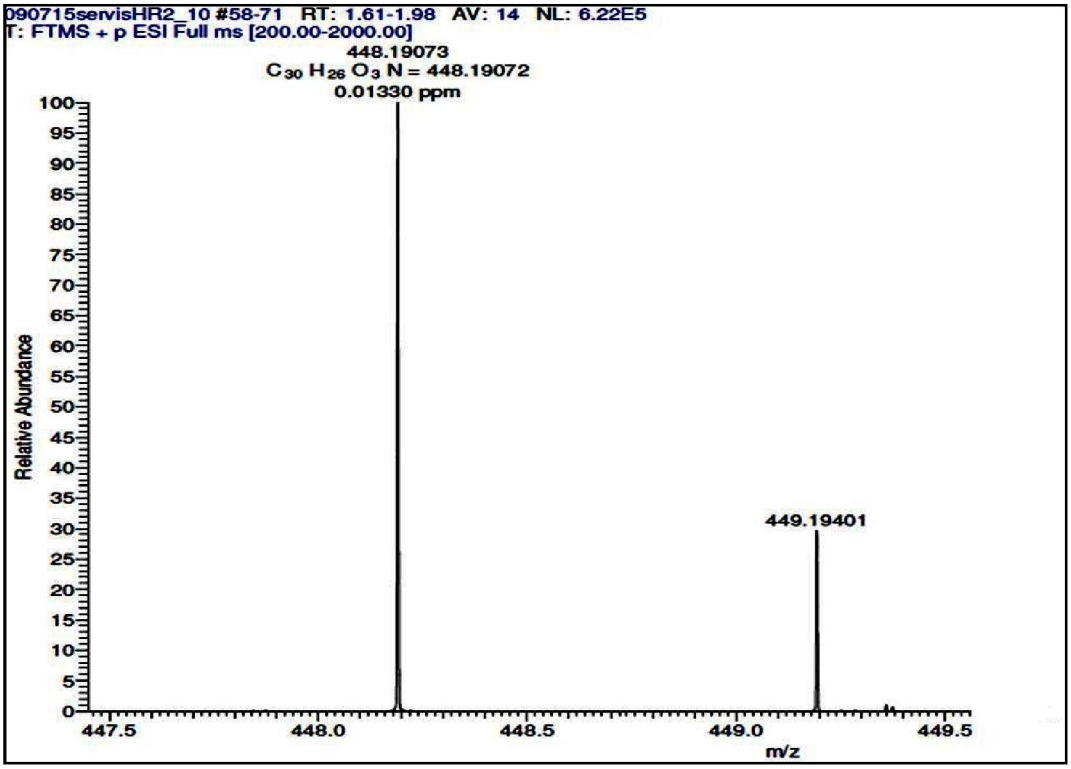


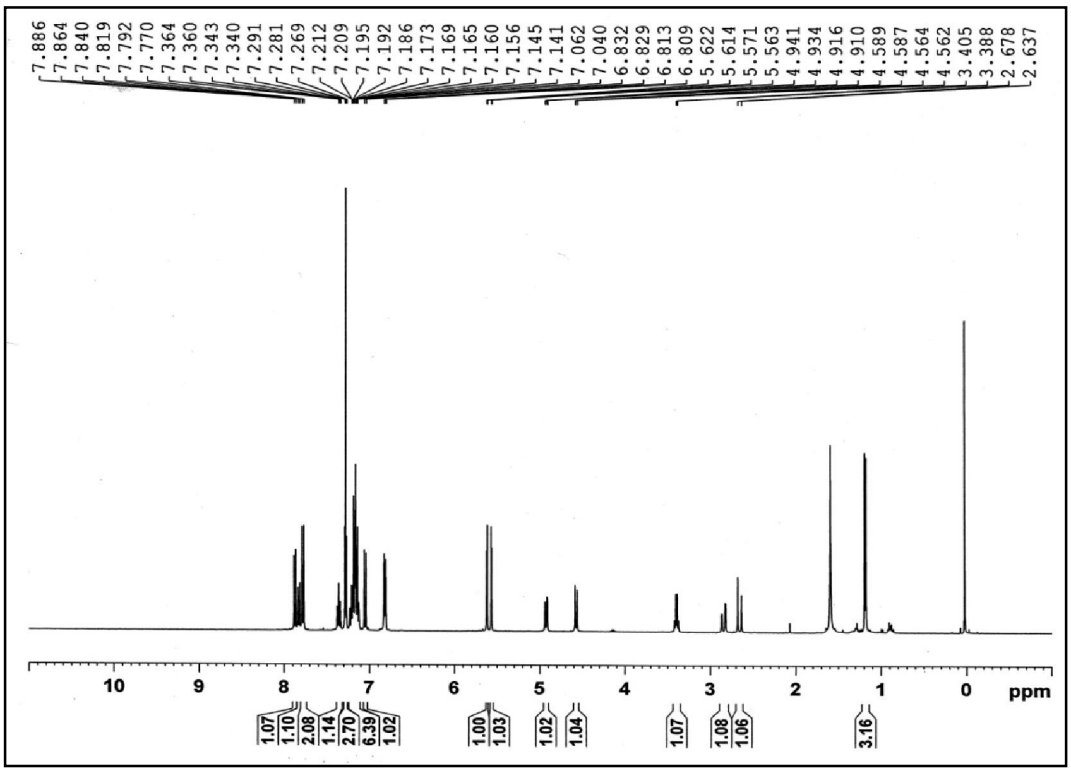
Figure 3: HPLC analysis of enantiomers pair of (*P*)-**11** and (*M*)-**11**



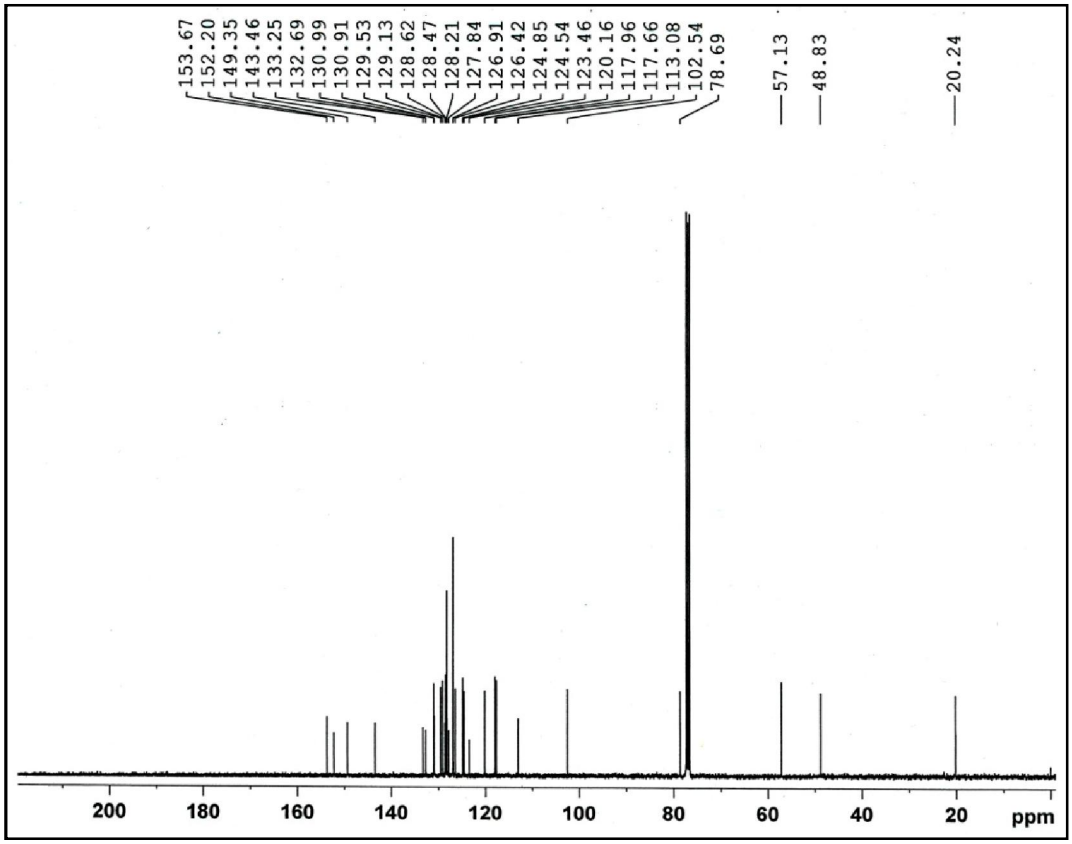
^{1}H-NMR Spectrum of compound (±)-12



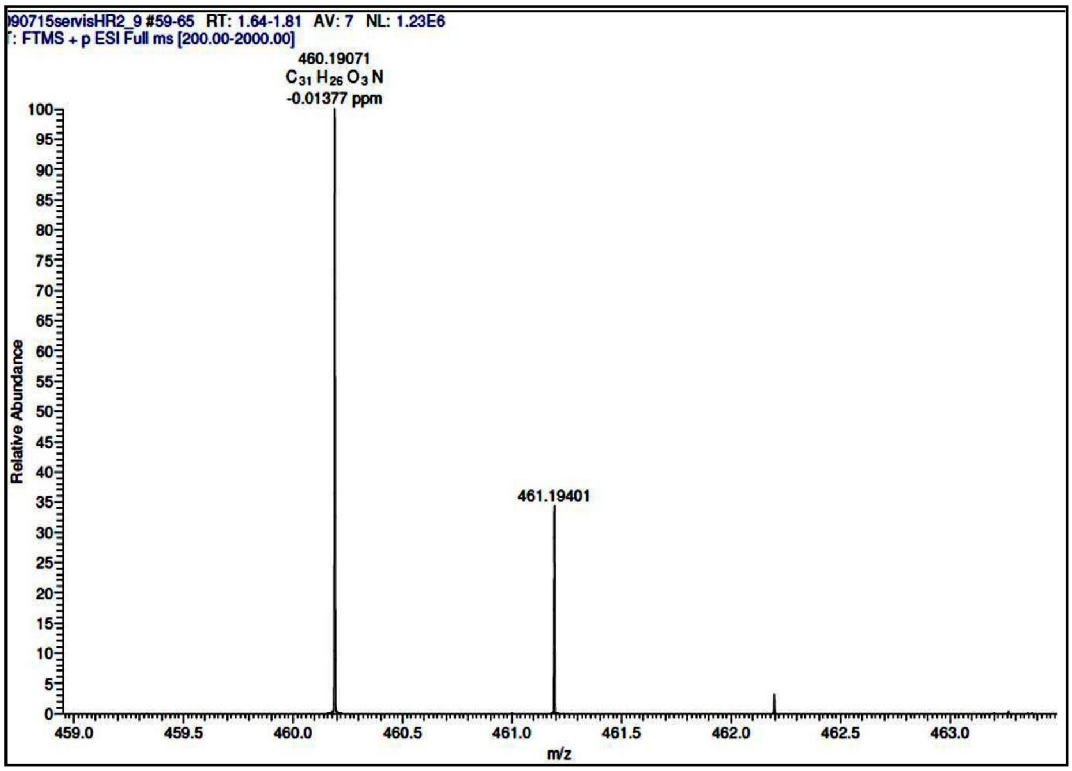
^{1}H-NMR Spectrum of compound (±)-12



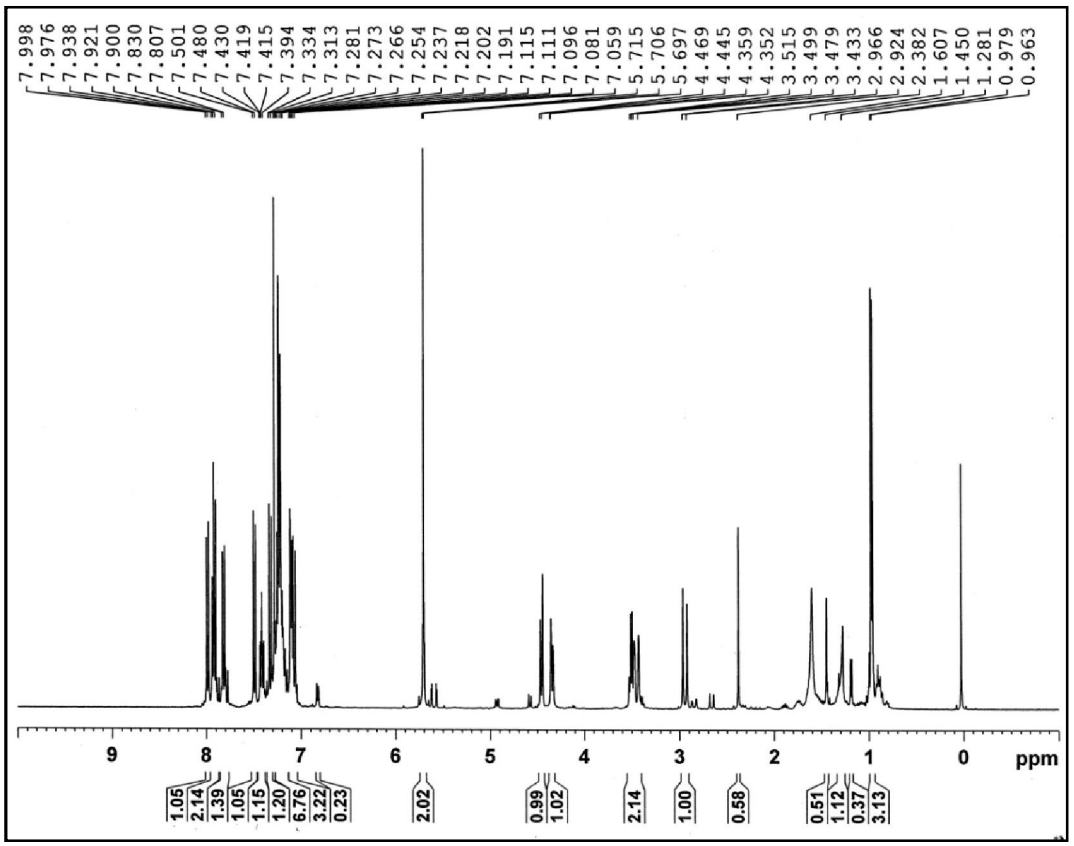
^{1}H-NMR Spectrum of compound [(*P*,*S*)-13]



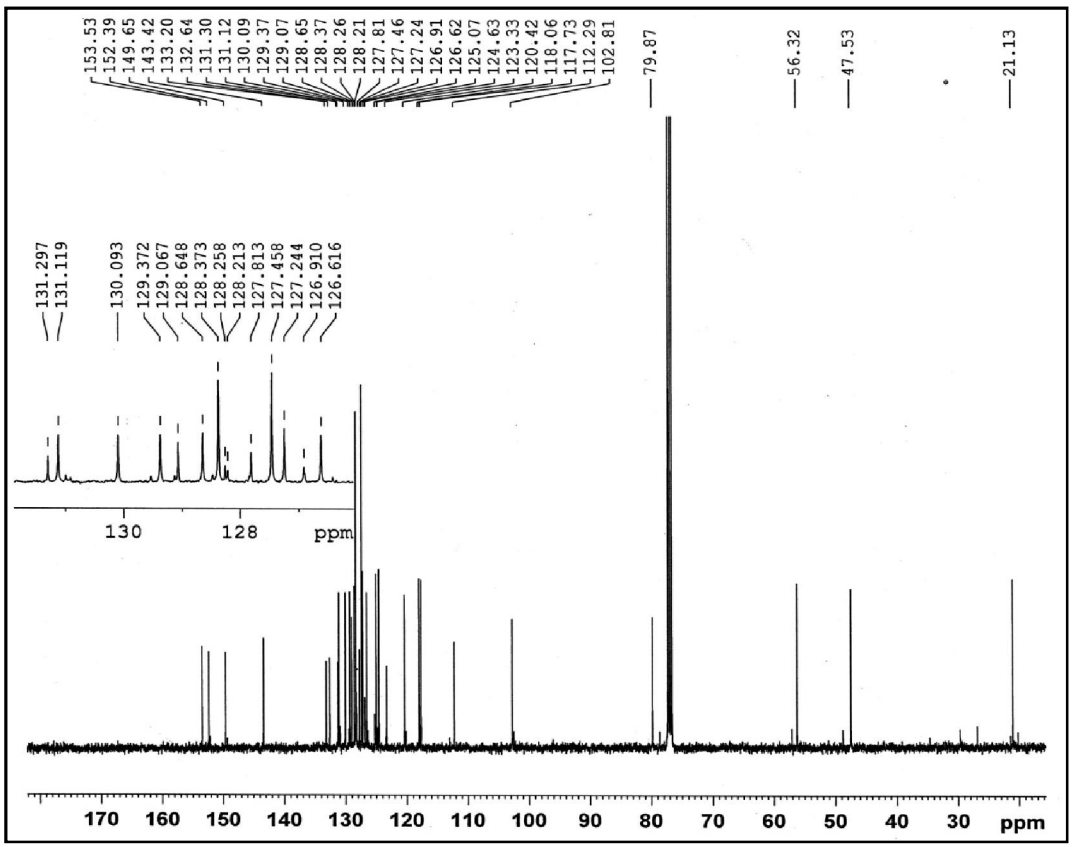
^{13}C-NMR spectrum of compound [(*P*,*S*)-13]



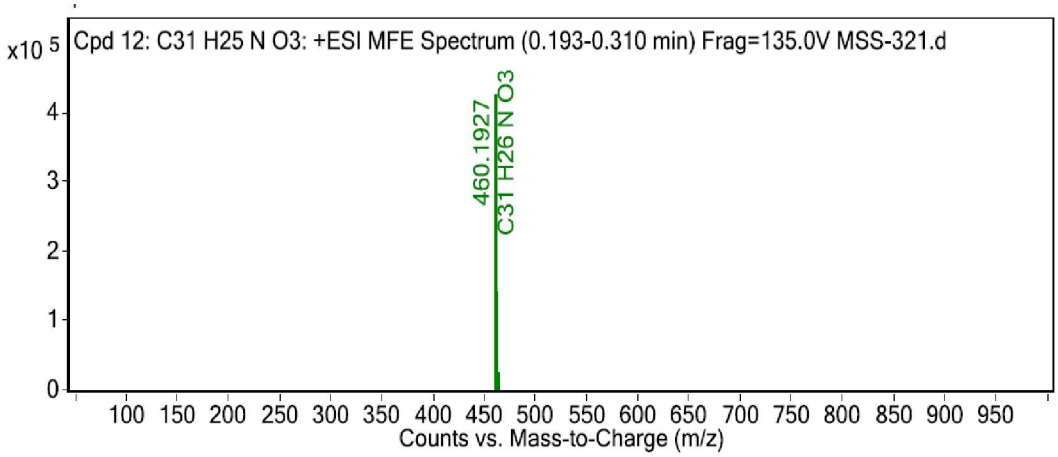
HRMS spectrum of compound [(*P*,*S*)-13]



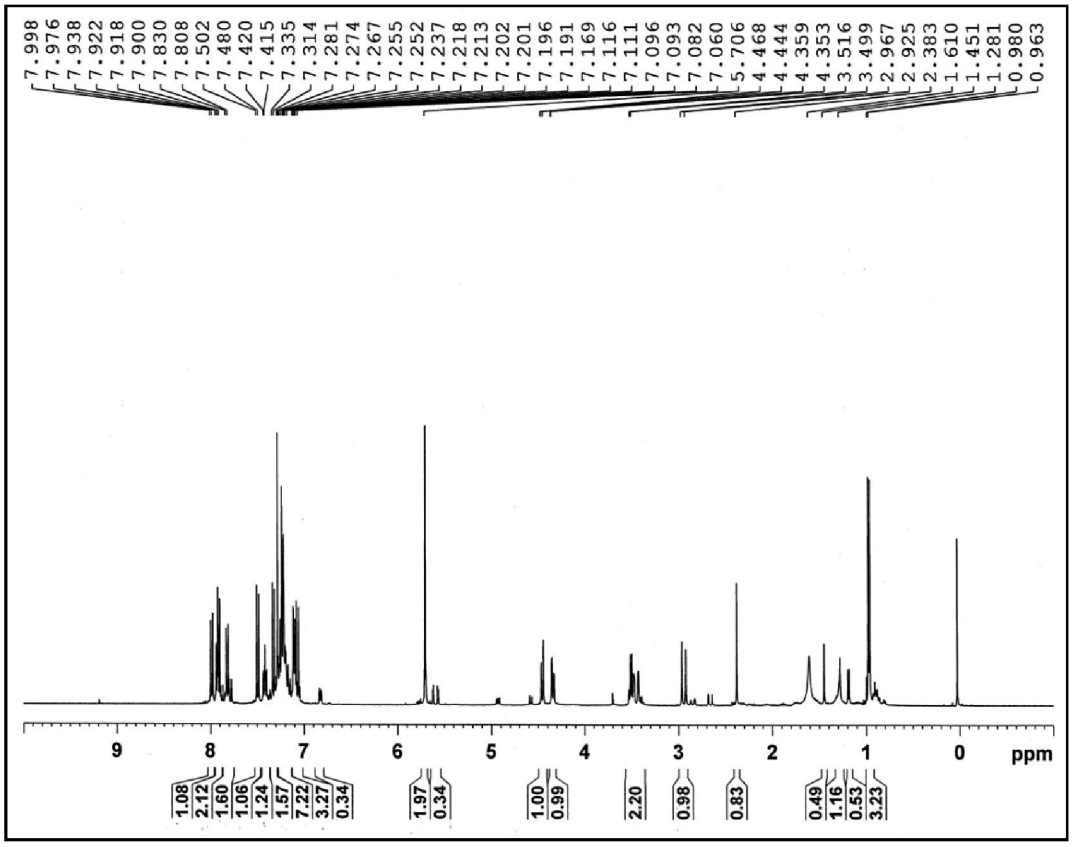
[1]H-NMR Spectrum of compound [(*P*,*R*)-13]



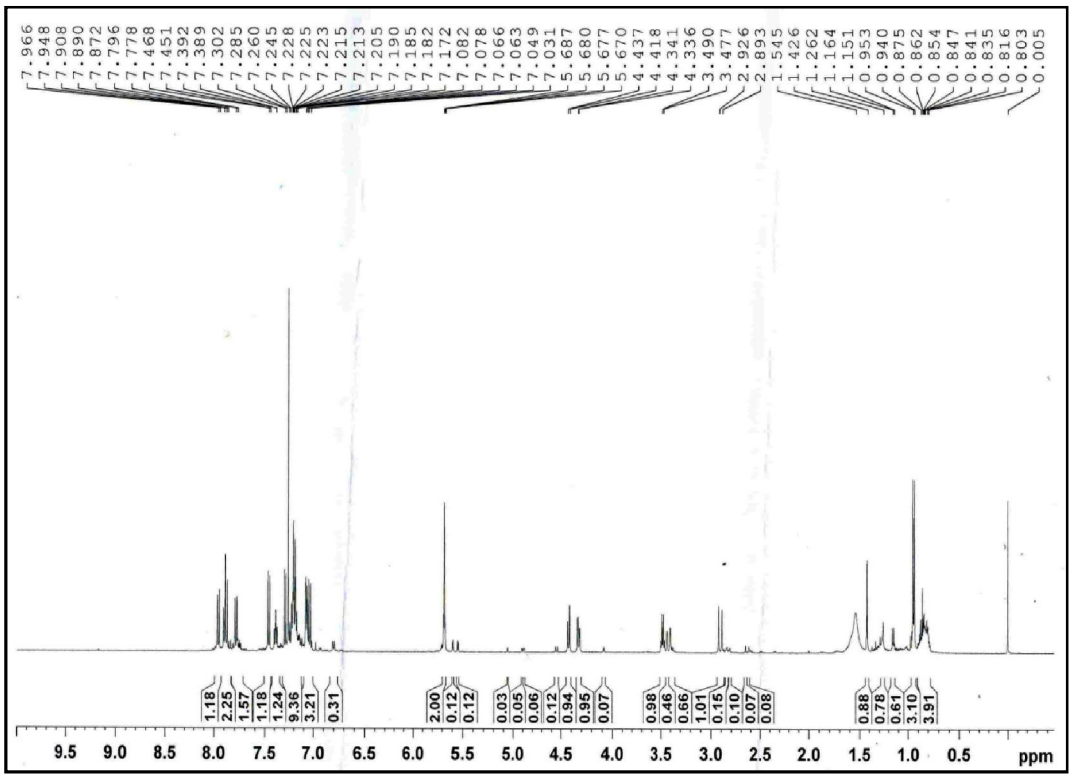
[13]C-NMR spectrum of compound [(*P*,*R*)-13]



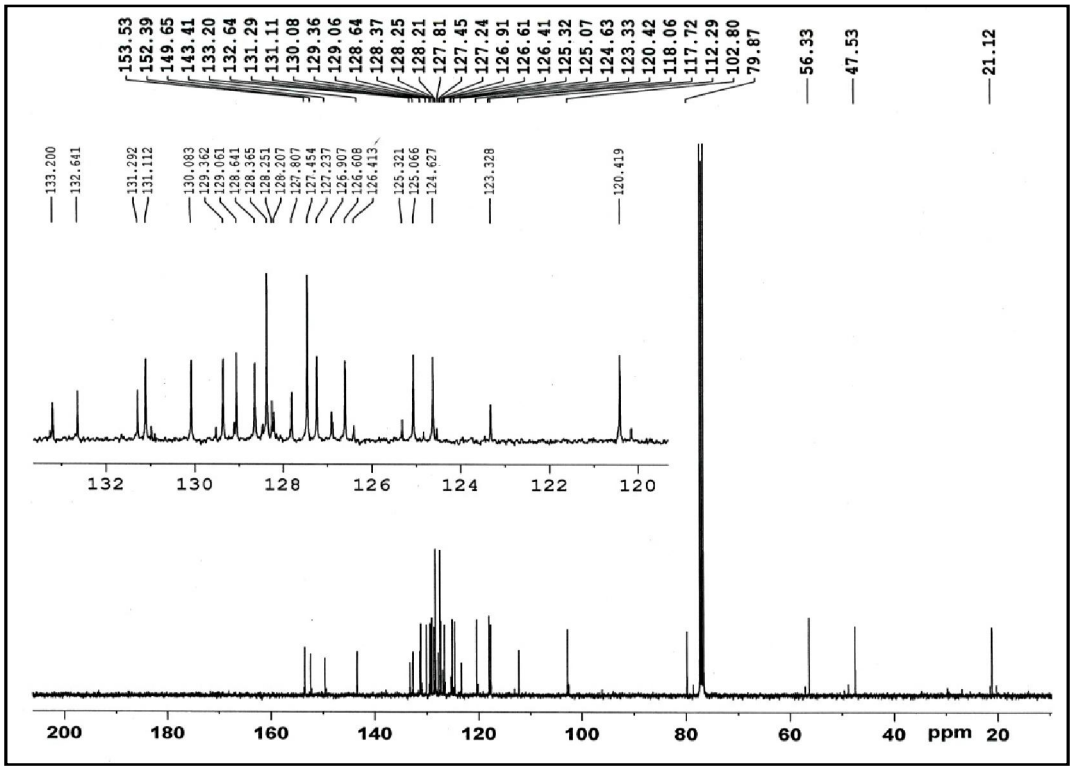
HRMS spectrum of compound [(*P*,*R*)-13]



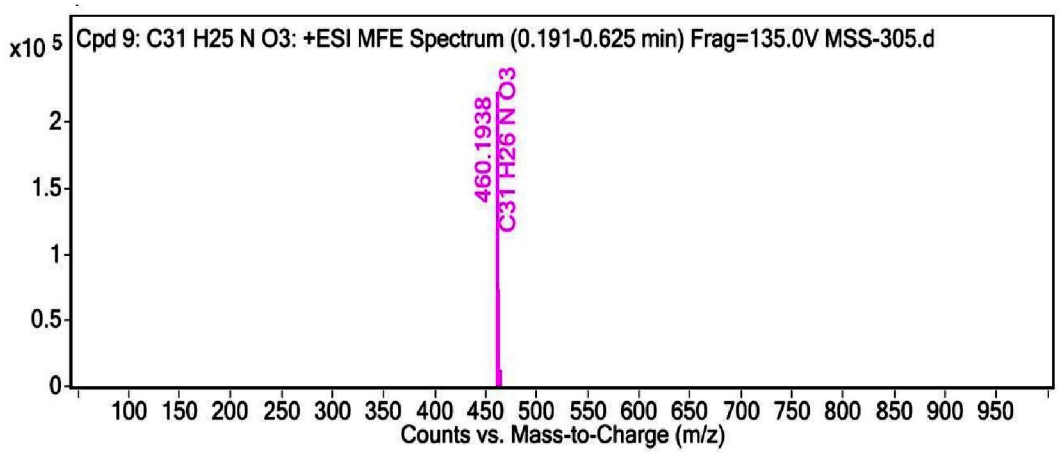
^{1}H-NMR Spectrum of compound [(*M*,*S*)-13]



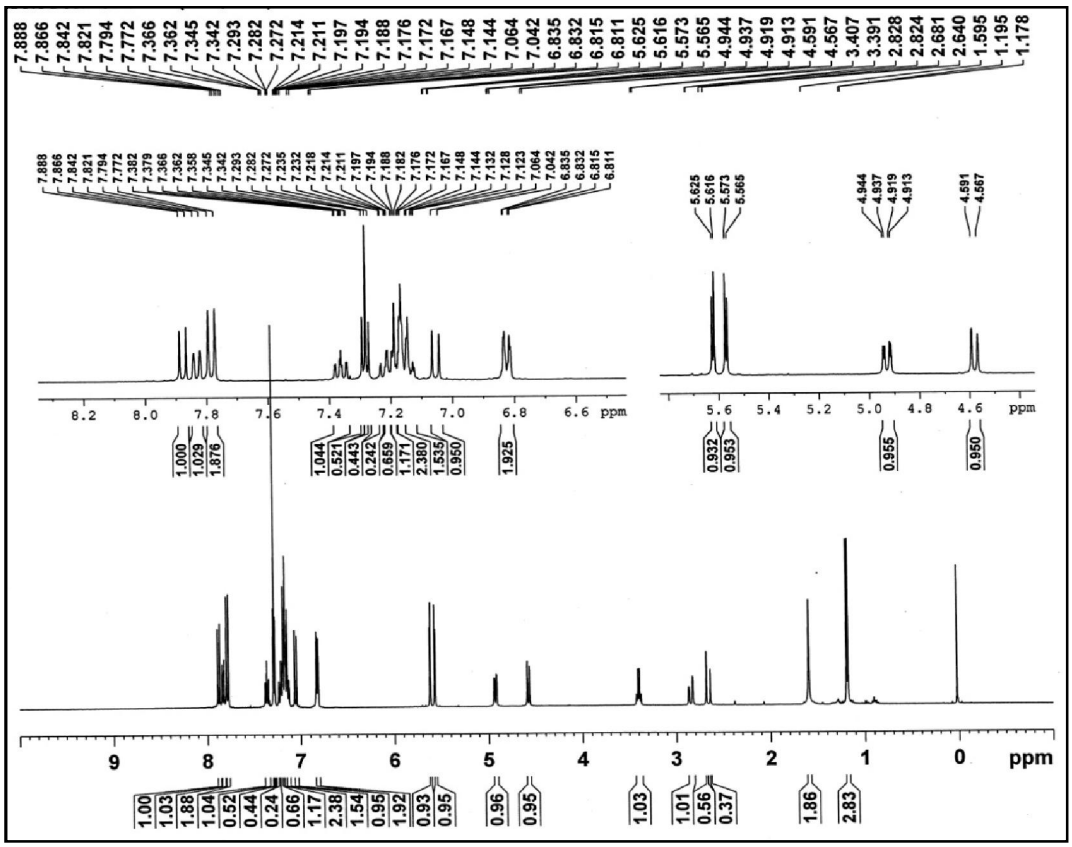
^{1}H-NMR Spectrum of compound [(*M*,*S*)-13]



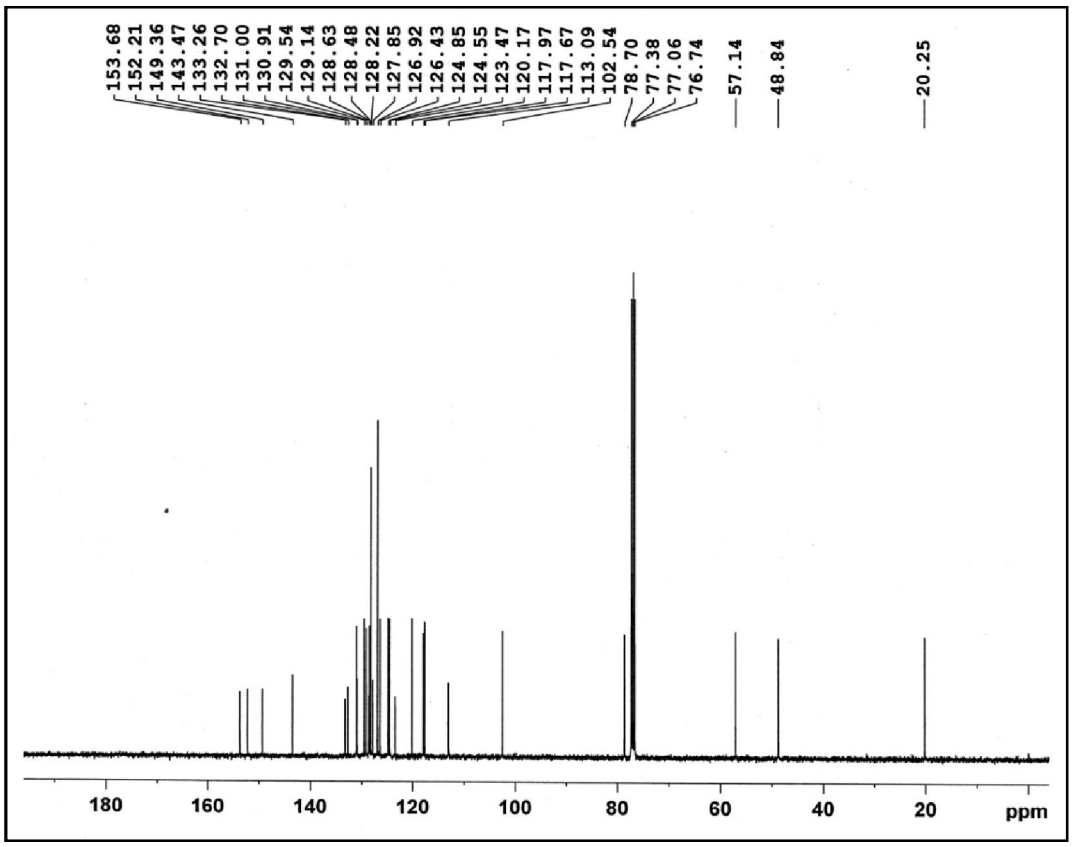
^{13}C-NMR spectrum of compound [(*M*,*S*)-13]



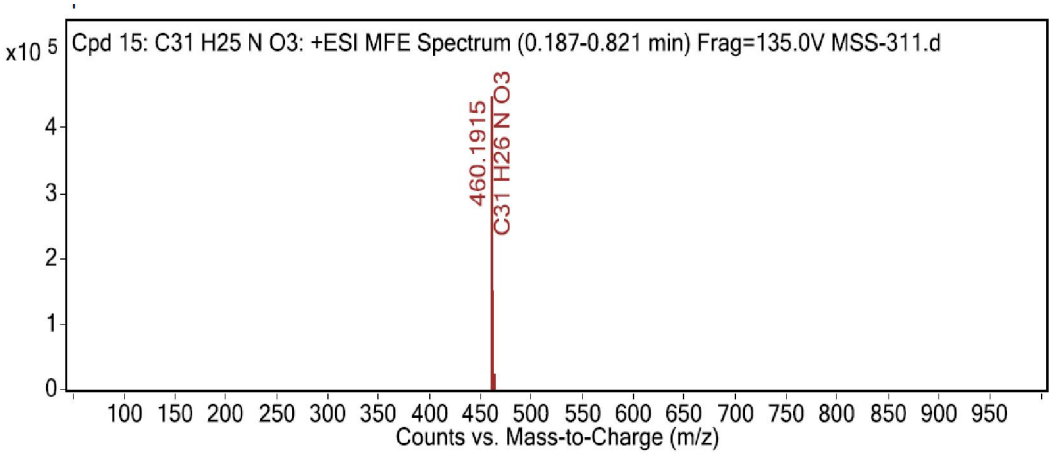
HRMS spectrum of compound [(*M*,*S*)-13]



^{1}H-NMR Spectrum of compound [(*M*,*R*)-13]



^{13}C-NMR spectrum of compound [(*M*,*R*)-13]



HRMS spectrum of compound [(*M*,*R*)-13]

1. **For the complex of (S_a)-1 and (*S*)-Brucine** (CCDC 1023827)**:**

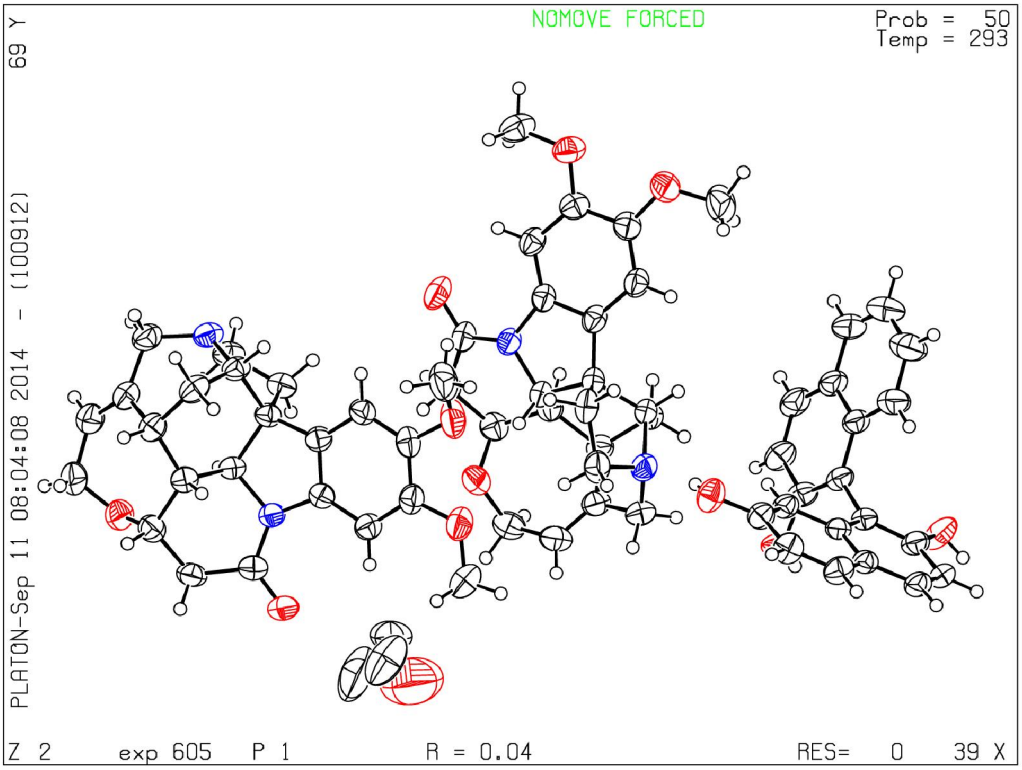


Figure 4: ORTEP diagram of the salt of (S_a)-**1**•(*S*)-Brucine with atom numbering scheme (50% probability factor for the thermal ellipsoids.

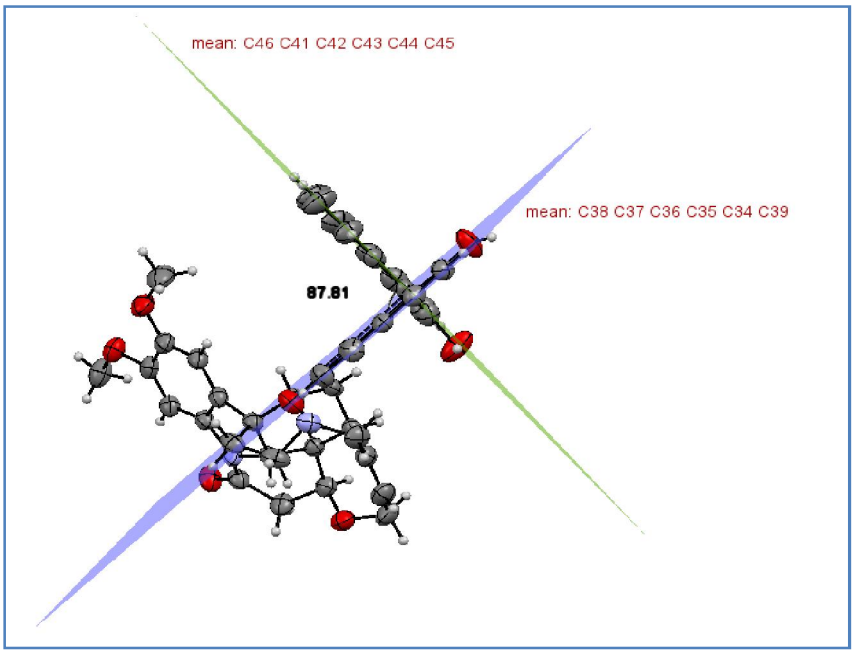


Figure 5: The planes passing through the molecule from the carbons C-46-C41-C42-C43-C44-C55 and C38-C37-C36-C35-C34-C39 showing the twist and the angle between the two planes are 87.81

In the X-ray diffraction analysis the angle between the planes passing through the two naphthalene rings and angle between the axis of the molecules was established. The stereochemistry of the axis clearly show the *S*-configuration by considering the known chirality in the molecule from the (*S*)-Brucine.

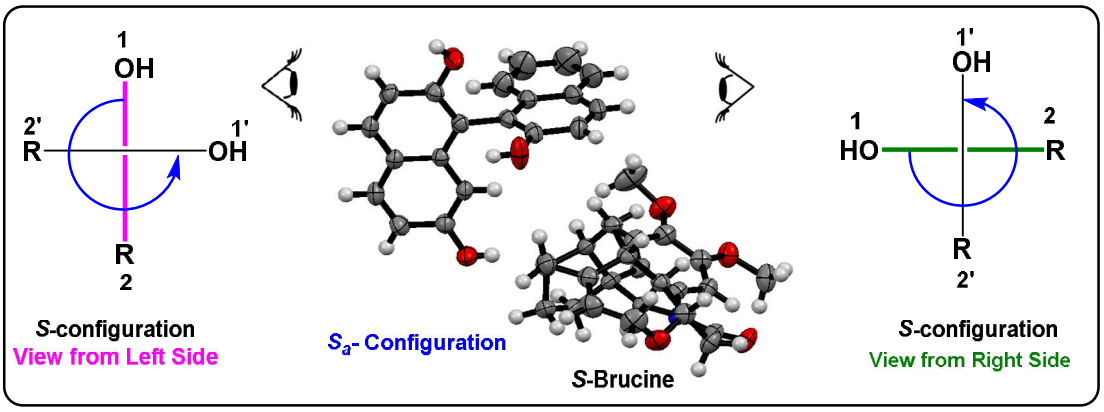


Figure 6: Configuration of the 1,1'-binaphthyl-2,2',7-triol (1) from the single crystal structure

Table 1 Crystal data and structure refinement for compound 1.

Empirical formula	$C_{67}H_{66}N_4O_{12}$
Formula weight	1119.24
Temperature/K	293(2)
Crystal system	triclinic
Space group	P1
a/Å	9.0356(2)
b/Å	10.3472(3)
c/Å	16.0067(5)
α/°	97.804(3)
β/°	104.923(2)
γ/°	100.186(2)
Volume/Å^3	1397.13(7)
Z	1
ρ_{calc}g/cm^3	1.330
μ/mm^{-1}	0.745
F(000)	592.0
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.84 to 146.1
Index ranges	$-9 \le h \le 11$, $-12 \le k \le 12$, $-19 \le l \le 19$
Reflections collected	14244
Independent reflections	7223 [R_{int} = 0.0340, R_{sigma} = 0.0333]
Data/restraints/parameters	7223/3/778
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0438, wR_2 = 0.1189

Final R indexes [all data] $R_1 = 0.0446$, $wR_2 = 0.1200$
Largest diff. peak/hole / e $Å^{-3}$ 0.20/-0.21
Flack parameter -0.06(15)

Table 2 Bond Lengths for compound 1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O29	C4	1.236(3)	C9	C10	1.391(4)
O51	C37	1.352(3)	C63	C61	1.512(4)
N5	C6	1.413(3)	C54	C59	1.387(3)
N5	C4	1.355(3)	C54	C55	1.395(3)
N5	C13	1.488(3)	C22	C12	1.542(3)
O75	C60	1.433(3)	C22	C21	1.517(4)
O75	C76	1.433(4)	C59	C58	1.391(3)
N65	C64	1.494(3)	C49	C48	1.419(3)
N65	C63	1.352(3)	C11	C12	1.504(3)
N65	C54	1.418(3)	C11	C10	1.394(3)
O50	C49	1.348(3)	C13	C14	1.526(3)
O27	C9	1.356(3)	C13	C12	1.560(3)
O27	C28	1.410(4)	C14	C19	1.540(3)
O25	C8	1.372(3)	C14	C2	1.532(3)
O25	C26	1.420(4)	C12	C23	1.532(4)
O18	C2	1.425(3)	C41	C46	1.425(4)
O18	C16	1.439(4)	C41	C42	1.411(4)
O79	C63	1.229(3)	C73	C72	1.521(4)
N71	C72	1.481(3)	C19	C17	1.526(3)
N71	C66	1.508(3)	C19	C21	1.530(3)
N71	C69	1.483(4)	C62	C60	1.537(3)
C39	C30	1.418(3)	C62	C68	1.533(3)
C39	C34	1.426(3)	C32	C33	1.358(4)
C39	C38	1.415(3)	C66	C70	1.514(4)
O52	C31	1.354(3)	C57	C58	1.392(4)
N20	C22	1.509(3)	C57	C56	1.405(4)
N20	C24	1.488(3)	C56	C55	1.384(4)
N20	C1	1.478(4)	C2	C3	1.539(4)
O77	C56	1.360(3)	C17	C15	1.319(4)
O77	C78	1.414(4)	C17	C1	1.511(4)
O80	C57	1.373(3)	C24	C23	1.510(4)
O80	C81	1.351(4)	C67	C68	1.524(4)
C6	C7	1.389(3)	C67	C69	1.507(4)
C6	C11	1.387(3)	C67	C74	1.321(4)
C31	C30	1.383(3)	C60	C61	1.548(4)
C31	C32	1.416(4)	C48	C47	1.349(4)
C64	C53	1.568(3)	C68	C70	1.535(4)
C64	C62	1.521(3)	C46	C47	1.404(5)
C4	C3	1.504(4)	C46	C45	1.422(4)

C40	C30	1.502(3)	C35	C36	1.356(4)
C40	C49	1.364(4)	C15	C16	1.494(5)
C40	C41	1.436(3)	C42	C43	1.375(4)
C53	C59	1.501(3)	C74	C76	1.499(4)
C53	C73	1.535(3)	C45	C44	1.352(7)
C53	C66	1.558(3)	C43	C44	1.387(7)
C7	C8	1.384(3)	O1	C5	1.228(15)
C37	C38	1.369(3)	O1	C82	1.350(19)
C37	C36	1.423(4)	O1	C18	1.380(16)
C34	C33	1.416(3)	C5	C82	1.26(3)
C34	C35	1.417(4)	C5	C18	1.07(2)
C9	C8	1.403(4)	C82	C18	1.30(3)

Table 3 Bond Angles for compound 1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C6	N5	C13	109.41(18)	C2	C14	C19	118.34(19)
C4	N5	C6	126.5(2)	C22	C12	C13	113.55(19)
C4	N5	C13	119.2(2)	C11	C12	C22	117.00(18)
C60	O75	C76	114.1(2)	C11	C12	C13	102.05(19)
C63	N65	C64	120.0(2)	C11	C12	C23	113.9(2)
C63	N65	C54	126.8(2)	C23	C12	C22	100.68(19)
C54	N65	C64	109.69(17)	C23	C12	C13	110.04(19)
C9	O27	C28	117.8(2)	C46	C41	C40	119.0(3)
C8	O25	C26	115.7(2)	C42	C41	C40	122.5(2)
C2	O18	C16	115.1(2)	C42	C41	C46	118.4(2)
C72	N71	C66	108.19(19)	C72	C73	C53	102.9(2)
C72	N71	C69	111.8(2)	C17	C19	C14	115.33(19)
C69	N71	C66	112.7(2)	C17	C19	C21	108.6(2)
C30	C39	C34	119.7(2)	C21	C19	C14	106.55(18)
C38	C39	C30	122.1(2)	C64	C62	C60	106.96(19)
C38	C39	C34	118.2(2)	C64	C62	C68	113.31(19)
C24	N20	C22	107.37(19)	C68	C62	C60	118.5(2)
C1	N20	C22	112.2(2)	C33	C32	C31	120.0(2)
C1	N20	C24	113.0(2)	N71	C72	C73	104.8(2)
C56	O77	C78	117.2(2)	N71	C66	C53	105.20(19)
C81	O80	C57	118.4(2)	N71	C66	C70	111.0(2)
C7	C6	N5	128.2(2)	C70	C66	C53	114.81(19)
C11	C6	N5	109.8(2)	O80	C57	C58	123.3(2)
C11	C6	C7	121.9(2)	O80	C57	C56	116.1(2)
O52	C31	C30	118.5(2)	C58	C57	C56	120.5(2)
O52	C31	C32	120.5(2)	C59	C58	C57	119.4(2)
C30	C31	C32	121.0(2)	O77	C56	C57	115.2(2)
N65	C64	C53	104.48(18)	O77	C56	C55	124.3(2)

N65	C64	C62	106.35(18)	C55	C56	C57	120.5(2)
C62	C64	C53	117.14(19)	O18	C2	C14	114.3(2)
O29	C4	N5	122.4(2)	O18	C2	C3	104.0(2)
O29	C4	C3	121.8(2)	C14	C2	C3	110.5(2)
N5	C4	C3	115.9(2)	C15	C17	C19	122.1(3)
C49	C40	C30	122.2(2)	C15	C17	C1	123.3(3)
C49	C40	C41	119.1(2)	C1	C17	C19	114.5(2)
C41	C40	C30	118.6(2)	N20	C24	C23	104.1(2)
C59	C53	C64	102.20(17)	C69	C67	C68	114.4(2)
C59	C53	C73	111.6(2)	C74	C67	C68	122.5(2)
C59	C53	C66	118.14(19)	C74	C67	C69	123.0(3)
C73	C53	C64	110.46(19)	O75	C60	C62	114.1(2)
C73	C53	C66	100.92(19)	O75	C60	C61	105.0(2)
C66	C53	C64	113.72(19)	C62	C60	C61	110.7(2)
C8	C7	C6	117.9(2)	C63	C61	C60	118.5(2)
O51	C37	C38	122.9(2)	C47	C48	C49	120.4(3)
O51	C37	C36	116.6(2)	C4	C3	C2	118.2(2)
C38	C37	C36	120.5(2)	C62	C68	C70	106.6(2)
C39	C30	C40	120.2(2)	C67	C68	C62	115.0(2)
C31	C30	C39	119.3(2)	C67	C68	C70	108.4(2)
C31	C30	C40	120.2(2)	C22	C21	C19	109.09(18)
C33	C34	C39	118.7(2)	C9	C10	C11	119.6(2)
C33	C34	C35	122.3(2)	C47	C46	C41	119.2(2)
C35	C34	C39	119.0(2)	C47	C46	C45	122.9(3)
C37	C38	C39	121.1(2)	C45	C46	C41	117.9(3)
O27	C9	C8	115.5(2)	C56	C55	C54	117.9(2)
O27	C9	C10	125.0(2)	N71	C69	C67	112.0(2)
C10	C9	C8	119.4(2)	C32	C33	C34	121.2(2)
N65	C63	C61	115.9(2)	C36	C35	C34	121.7(2)
O79	C63	N65	123.1(2)	C24	C23	C12	102.2(2)
O79	C63	C61	121.0(2)	C66	C70	C68	109.3(2)
C59	C54	N65	109.6(2)	C17	C15	C16	122.3(3)
C59	C54	C55	122.5(2)	C35	C36	C37	119.4(2)
C55	C54	N65	127.9(2)	C48	C47	C46	121.1(2)
O25	C8	C7	124.2(2)	C43	C42	C41	121.1(3)
O25	C8	C9	114.5(2)	C67	C74	C76	122.3(3)
C7	C8	C9	121.4(2)	O18	C16	C15	111.2(3)
N20	C22	C12	105.27(19)	N20	C1	C17	111.9(2)
N20	C22	C21	112.0(2)	O75	C76	C74	112.1(2)
C21	C22	C12	114.2(2)	C44	C45	C46	122.0(3)
C54	C59	C53	111.51(19)	C42	C43	C44	120.6(4)
C54	C59	C58	119.1(2)	C45	C44	C43	120.0(3)
C58	C59	C53	129.1(2)	C5	O1	C82	58.2(13)
O50	C49	C40	124.8(2)	C5	O1	C18	48.0(12)
O50	C49	C48	114.1(3)	C82	O1	C18	56.9(14)

C40	C49	C48	121.1(2)	O1	C5	C82	65.7(11)
C6	C11	C12	110.7(2)	C18	C5	O1	73.5(13)
C6	C11	C10	119.5(2)	C18	C5	C82	67.3(19)
C10	C11	C12	129.7(2)	C5	C82	O1	56.1(12)
N5	C13	C14	105.89(18)	C5	C82	C18	49.4(15)
N5	C13	C12	104.24(18)	C18	C82	O1	62.8(12)
C14	C13	C12	117.43(18)	C5	C18	O1	58.6(10)
C13	C14	C19	112.11(19)	C5	C18	C82	63.3(19)
C13	C14	C2	107.48(19)	C82	C18	O1	60.4(11)

Table 4 Torsion Angles for compound 1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O29	C4	C3	C2	145.7(3)	C13	C14	C19	C17	60.6(3)
O51	C37	C38	C39	-179.2(2)	C13	C14	C19	C21	-60.0(2)
O51	C37	C36	C35	179.3(3)	C13	C14	C2	O18	-74.4(2)
N5	C6	C7	C8	-175.5(2)	C13	C14	C2	C3	42.5(3)
N5	C6	C11	C12	-8.2(3)	C13	C12	C23	C24	75.9(2)
N5	C6	C11	C10	175.4(2)	C14	C13	C12	C22	-29.0(3)
N5	C4	C3	C2	-34.2(4)	C14	C13	C12	C11	97.8(2)
N5	C13	C14	C19	157.28(18)	C14	C13	C12	C23	-140.9(2)
N5	C13	C14	C2	-71.0(2)	C14	C19	C17	C15	59.3(3)
N5	C13	C12	C22	-145.7(2)	C14	C19	C17	C1	-118.2(3)
N5	C13	C12	C11	-18.9(2)	C14	C19	C21	C22	68.7(2)
N5	C13	C12	C23	102.3(2)	C14	C2	C3	C4	8.3(4)
O75	C60	C61	C63	127.6(2)	C12	C22	C21	C19	-58.6(2)
N65	C64	C53	C59	-15.2(2)	C12	C11	C10	C9	-176.3(2)
N65	C64	C53	C73	103.7(2)	C12	C13	C14	C19	41.4(3)
N65	C64	C53	C66	143.68(19)	C12	C13	C14	C2	173.1(2)
N65	C64	C62	C60	-70.9(2)	C41	C40	C30	C39	89.3(3)
N65	C64	C62	C68	156.68(19)	C41	C40	C30	C31	-85.1(3)
N65	C63	C61	C60	-30.5(4)	C41	C40	C49	O50	-176.8(3)
N65	C54	C59	C53	-8.3(3)	C41	C40	C49	C48	2.0(4)
N65	C54	C59	C58	176.8(2)	C41	C46	C47	C48	0.2(4)
N65	C54	C55	C56	-177.3(2)	C41	C46	C45	C44	1.1(5)
O50	C49	C48	C47	177.2(3)	C41	C42	C43	C44	0.5(7)
O27	C9	C8	O25	-1.6(3)	C73	C53	C59	C54	-103.3(2)
O27	C9	C8	C7	177.7(2)	C73	C53	C59	C58	71.1(3)
O27	C9	C10	C11	-178.6(3)	C73	C53	C66	N71	30.7(2)
O18	C2	C3	C4	131.4(3)	C73	C53	C66	C70	153.1(2)
O79	C63	C61	C60	150.1(3)	C19	C14	C2	O18	53.8(3)
N71	C66	C70	C68	62.3(2)	C19	C14	C2	C3	170.7(2)
C39	C34	C33	C32	-1.4(3)	C19	C17	C15	C16	-3.5(5)
C39	C34	C35	C36	0.6(4)	C19	C17	C1	N20	52.4(3)

O52 C31 C30 C39	180.0(2)	C62 C64 C53 C59	102.1(2)
O52 C31 C30 C40	-5.6(4)	C62 C64 C53 C73	-139.0(2)
O52 C31 C32 C33	178.4(2)	C62 C64 C53 C66	-26.4(3)
N20 C22 C12 C11	155.4(2)	C62 C60 C61 C63	4.1(3)
N20 C22 C12 C13	-86.0(2)	C62 C68 C70 C66	68.1(2)
N20 C22 C12 C23	31.5(2)	C32 C31 C30 C39	-2.1(3)
N20 C22 C21 C19	61.0(2)	C32 C31 C30 C40	172.3(2)
N20 C24 C23 C12	40.9(2)	C72 N71 C66 C53	-8.0(2)
O77 C56 C55 C54	-178.8(2)	C72 N71 C66 C70	-132.8(2)
O80 C57 C58 C59	-179.3(2)	C72 N71 C69 C67	74.6(3)
O80 C57 C56 O77	-1.6(4)	C66 N71 C72 C73	-18.4(2)
O80 C57 C56 C55	178.5(2)	C66 N71 C69 C67	-47.5(3)
C6 N5 C4 O29	-23.3(4)	C66 C53 C59 C54	140.4(2)
C6 N5 C4 C3	156.6(2)	C66 C53 C59 C58	-45.3(4)
C6 N5 C13 C14	-109.0(2)	C66 C53 C73 C72	-41.8(2)
C6 N5 C13 C12	15.5(2)	C57 C56 C55 C54	1.1(4)
C6 C7 C8 O25	-179.1(2)	C58 C57 C56 O77	176.5(2)
C6 C7 C8 C9	1.7(4)	C58 C57 C56 C55	-3.4(4)
C6 C11 C12 C22	141.6(2)	C56 C57 C58 C59	2.7(4)
C6 C11 C12 C13	17.0(3)	C2 O18 C16 C15	89.6(3)
C6 C11 C12 C23	-101.5(2)	C2 C14 C19 C17	-65.4(3)
C6 C11 C10 C9	-0.6(4)	C2 C14 C19 C21	174.0(2)
C31 C32 C33 C34	1.3(4)	C17 C19 C21 C22	-56.1(2)
C64 N65 C63 O79	-177.4(3)	C17 C15 C16 O18	-64.3(4)
C64 N65 C63 C61	3.2(3)	C24 N20 C22 C12	-7.0(3)
C64 N65 C54 C59	-2.6(3)	C24 N20 C22 C21	-131.7(2)
C64 N65 C54 C55	176.7(2)	C24 N20 C1 C17	73.1(3)
C64 C53 C59 C54	14.8(3)	C67 C68 C70 C66	-56.2(2)
C64 C53 C59 C58	-170.9(2)	C67 C74 C76 O75	-65.0(4)
C64 C53 C73 C72	78.8(2)	C60 O75 C76 C74	88.8(3)
C64 C53 C66 N71	-87.6(2)	C60 C62 C68 C67	-66.5(3)
C64 C53 C66 C70	34.8(3)	C60 C62 C68 C70	173.4(2)
C64 C62 C60 O75	-73.2(3)	C68 C62 C60 O75	56.3(3)
C64 C62 C60 C61	44.9(3)	C68 C62 C60 C61	174.4(2)
C64 C62 C68 C67	60.1(3)	C68 C67 C69 N71	52.8(3)
C64 C62 C68 C70	-60.1(3)	C68 C67 C74 C76	-2.3(4)
C4 N5 C6 C7	17.7(4)	C21 C22 C12 C11	-81.3(3)
C4 N5 C6 C11	-160.0(2)	C21 C22 C12 C13	37.2(3)
C4 N5 C13 C14	47.9(3)	C21 C22 C12 C23	154.8(2)
C4 N5 C13 C12	172.4(2)	C21 C19 C17 C15	178.7(3)
C40 C49 C48 C47	-1.8(4)	C21 C19 C17 C1	1.2(3)
C40 C41 C46 C47	0.1(4)	C10 C9 C8 O25	176.0(2)
C40 C41 C46 C45	179.3(3)	C10 C9 C8 C7	-4.7(4)
C40 C41 C42 C43	179.9(4)	C10 C11 C12 C22	-42.4(4)
C53 C64 C62 C60	172.76(19)	C10 C11 C12 C13	-167.0(3)

C53 C64 C62 C68	40.4(3)	C10 C11 C12 C23	74.5(3)
C53 C59 C58 C57	-173.8(2)	C46 C41 C42 C43	-0.3(5)
C53 C73 C72 N71	38.0(2)	C46 C45 C44 C43	-0.9(7)
C53 C66 C70 C68	-56.9(3)	C55 C54 C59 C53	172.4(2)
C7 C6 C11 C12	174.0(2)	C55 C54 C59 C58	-2.6(4)
C7 C6 C11 C10	-2.5(4)	C69 N71 C72 C73	-143.0(2)
C30 C39 C34 C33	-0.2(3)	C69 N71 C66 C53	116.0(2)
C30 C39 C34 C35	178.7(2)	C69 N71 C66 C70	-8.7(3)
C30 C39 C38 C37	-179.6(2)	C69 C67 C68 C62	-119.1(3)
C30 C31 C32 C33	0.5(4)	C69 C67 C68 C70	0.1(3)
C30 C40 C49 O50	1.9(4)	C69 C67 C74 C76	174.2(3)
C30 C40 C49 C48	-179.3(2)	C33 C34 C35 C36	179.5(2)
C30 C40 C41 C46	-179.9(2)	C35 C34 C33 C32	179.7(2)
C30 C40 C41 C42	-0.1(4)	C15 C17 C1 N20	-125.0(3)
C34 C39 C30 C31	2.0(3)	C36 C37 C38 C39	1.2(4)
C34 C39 C30 C40	-172.5(2)	C47 C46 C45 C44	-179.7(4)
C34 C39 C38 C37	-0.4(3)	C42 C41 C46 C47	-179.8(3)
C34 C35 C36 C37	0.2(4)	C42 C41 C46 C45	-0.5(4)
C38 C39 C30 C31	-178.9(2)	C42 C43 C44 C45	0.1(8)
C38 C39 C30 C40	6.7(3)	C26 O25 C8 C7	-3.3(4)
C38 C39 C34 C33	-179.4(2)	C26 O25 C8 C9	176.0(3)
C38 C39 C34 C35	-0.5(3)	C74 C67 C68 C62	57.8(3)
C38 C37 C36 C35	-1.1(4)	C74 C67 C68 C70	176.9(3)
C63 N65 C64 C53	171.9(2)	C74 C67 C69 N71	-124.0(3)
C63 N65 C64 C62	47.3(3)	C16 O18 C2 C14	-67.3(3)
C63 N65 C54 C59	-161.2(2)	C16 O18 C2 C3	172.1(2)
C63 N65 C54 C55	18.1(4)	C1 N20 C22 C12	117.7(2)
C54 N65 C64 C53	11.6(2)	C1 N20 C22 C21	-7.0(3)
C54 N65 C64 C62	-113.0(2)	C1 N20 C24 C23	-145.1(2)
C54 N65 C63 O79	-20.8(4)	C1 C17 C15 C16	173.7(3)
C54 N65 C63 C61	159.9(2)	C28 O27 C9 C8	-171.0(3)
C54 C59 C58 C57	0.2(4)	C28 O27 C9 C10	11.6(5)
C8 C9 C10 C11	4.1(4)	C78 O77 C56 C57	-178.9(3)
C22 N20 C24 C23	-20.9(3)	C78 O77 C56 C55	1.0(4)
C22 N20 C1 C17	-48.4(3)	C76 O75 C60 C62	-67.7(3)
C22 C12 C23 C24	-44.2(2)	C76 O75 C60 C61	171.0(2)
C59 C53 C73 C72	−168.17(18)	C45 C46 C47 C48	-179.0(3)
C59 C53 C66 N71	152.6(2)	C81 O80 C57 C58	44.3(5)
C59 C53 C66 C70	-85.0(3)	C81 O80 C57 C56	-137.6(4)
C59 C54 C55 C56	1.9(4)	O1 C5 C82 C18	81.4(15)
C49 C40 C30 C39	-89.4(3)	O1 C5 C18 C82	-70.0(11)
C49 C40 C30 C31	96.2(3)	O1 C82 C18 C5	67.3(14)
C49 C40 C41 C46	-1.2(3)	C5 O1 C82 C18	-57.6(15)
C49 C40 C41 C42	178.6(3)	C5 O1 C18 C82	75(2)

C49	C48	C47	C46	0.6(5)	C5	C82	C18 O1	-67.3(14)
C11	C6	C7	C8	1.9(4)	C82	O1	C5 C18	72(2)
C11	C12	C23	C24	170.30(19)	C82	O1	C18 C5	-75(2)
C13	N5	C6	C7	172.5(2)	C82	C5	C18 O1	70.0(11)
C13	N5	C6	C11	-5.2(3)	C18	O1	C5 C82	-72(2)
C13	N5	C4	O29	-175.9(2)	C18	O1	C82 C5	57.6(15)
C13	N5	C4	C3	3.9(3)	C18	C5	C82 O1	-81.4(15)

2. **For compound** (*P*)-**9** (CCDC 1453552):

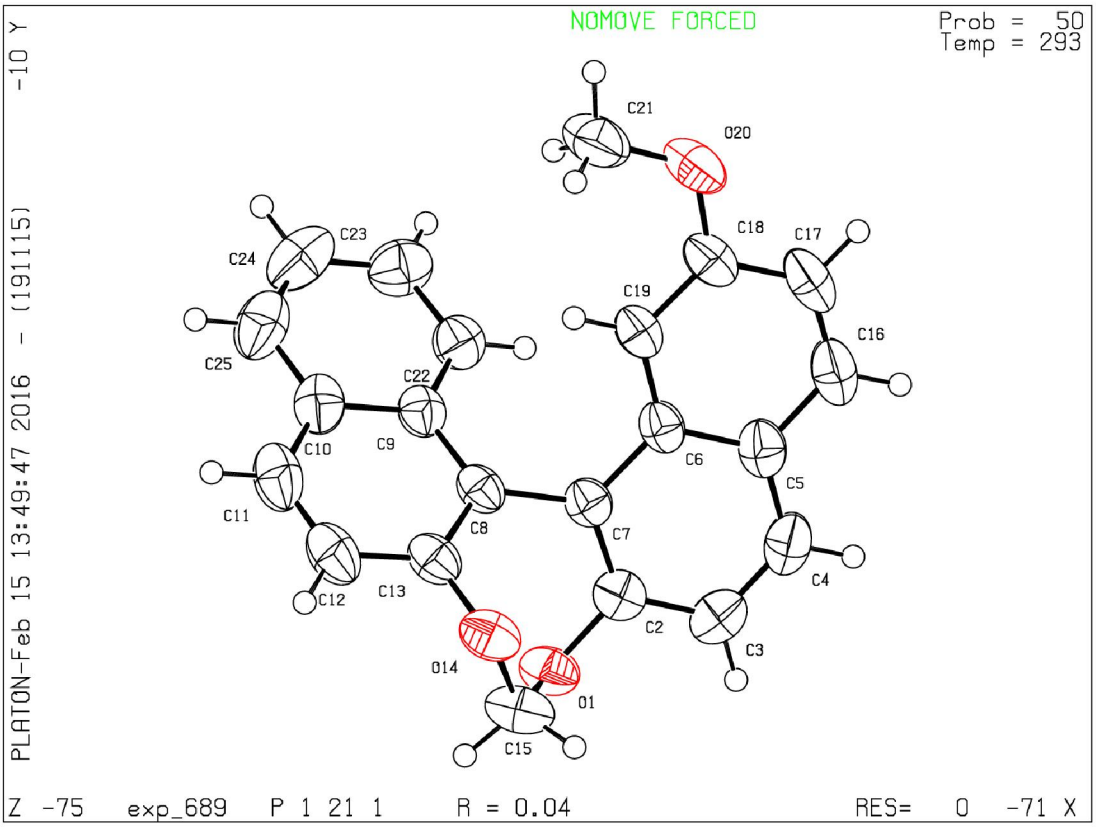


Figure 7: ORTEP diagram of (*P*)-**9**. Hydrogens are omitted for clarity with atom numbering scheme (50% probability factor for the thermal ellipsoids).

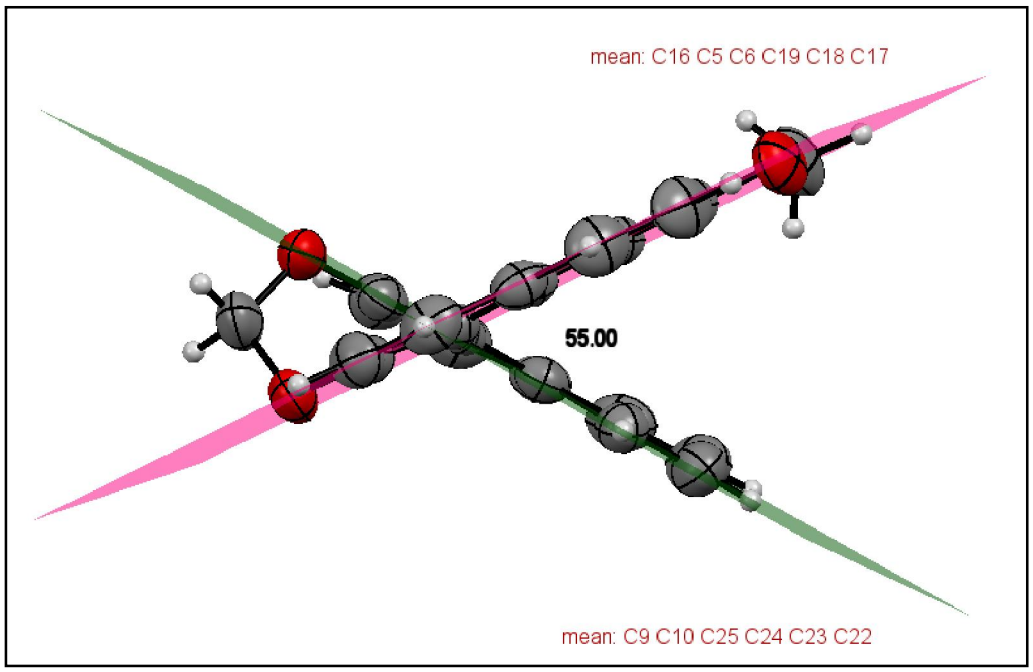


Figure 8: The planes passing through the molecule from the carbons C-16-C5-C6-C19-C18-C17 and C9-C10-C25-C24-C23-C22 showing the twist and the angle between the two planes are 55.0

Table 5 Crystal data and structure refinement for compound (*P*)-**9.**

Empirical formula	$C_{23}H_{17}O_2$
Formula weight	328.35
Temperature/K	293
Crystal system	monoclinic
Space group	$P2_1$
a/Å	9.9608(3)
b/Å	9.4348(3)
c/Å	10.0343(3)
α/°	90
β/°	113.748(4)
γ/°	90
Volume/Å^3	863.16(5)
Z	2
ρ_{calc}g/cm^3	1.2633
μ/mm^{-1}	0.672
F(000)	344.0
2Θ range for data collection/°	9.62 to 146.2
Index ranges	$-12 \leq h \leq 12$, $-11 \leq k \leq 9$, $-12 \leq l \leq 12$
Reflections collected	9817
Independent reflections	2967 [R_{int} = 0.0232, R_{sigma} = 0.0208]
Data/restraints/parameters	2967/0/226
Goodness-of-fit on F^2	0.637
Final R indexes [I>=2σ (I)]	R_1 = 0.0366
Final R indexes [all data]	R_1 = 0.0391, wR_2 = 0.1175

Largest diff. peak/hole / e Å^{-3}	0.16/-0.15
Flack parameter	0.1(2)

Table 6 Bond Lengths for Compound (*P*)-9.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C2	1.393(2)	C13	C12	1.401(3)
O1	C15	1.406(3)	C9	C22	1.412(3)
O14	C13	1.385(2)	C9	C10	1.431(2)
O14	C15	1.411(3)	C4	C3	1.358(3)
C7	C8	1.486(2)	C4	C5	1.410(3)
C7	C6	1.431(2)	C18	C17	1.411(3)
C7	C2	1.377(2)	C22	C23	1.370(3)
O20	C18	1.363(3)	C10	C11	1.416(3)
O20	C21	1.411(3)	C10	C25	1.414(3)
C8	C13	1.378(2)	C5	C16	1.420(3)
C8	C9	1.424(2)	C11	C12	1.354(3)
C6	C19	1.416(2)	C25	C24	1.345(4)
C6	C5	1.422(2)	C23	C24	1.410(4)
C2	C3	1.404(3)	C16	C17	1.352(4)
C19	C18	1.371(2)			

Table 7 Bond Angles for compound (*P*)-9.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C15	O1	C2	112.94(15)	C10	C9	C22	117.83(16)
C15	O14	C13	114.89(16)	C5	C4	C3	120.96(18)
C6	C7	C8	124.20(15)	C19	C18	O20	124.73(18)
C2	C7	C8	117.70(14)	C17	C18	O20	114.86(16)
C2	C7	C6	118.07(15)	C17	C18	C19	120.40(19)
C21	O20	C18	117.00(14)	C23	C22	C9	121.3(2)
C13	C8	C7	117.61(15)	C4	C3	C2	118.82(18)
C9	C8	C7	123.76(14)	C11	C10	C9	119.10(18)
C9	C8	C13	118.51(15)	C25	C10	C9	118.83(19)
C19	C6	C7	122.23(15)	C25	C10	C11	122.06(19)
C5	C6	C7	118.57(16)	C4	C5	C6	120.11(17)
C5	C6	C19	119.19(15)	C16	C5	C6	118.10(19)
C7	C2	O1	118.77(16)	C16	C5	C4	121.79(19)
C3	C2	O1	117.92(17)	C12	C11	C10	121.34(18)
C3	C2	C7	123.29(17)	C11	C12	C13	119.28(18)
C18	C19	C6	120.42(17)	C24	C25	C10	121.6(2)
C8	C13	O14	119.50(16)	C24	C23	C22	120.1(2)
C12	C13	O14	117.70(16)	O14	C15	O1	112.82(14)
C12	C13	C8	122.71(18)	C17	C16	C5	121.72(19)
C22	C9	C8	123.28(16)	C16	C17	C18	120.08(17)
C10	C9	C8	118.85(16)	C23	C24	C25	120.2(2)

3. For compound (*P*,*S*)-**13** (CCDC 1041059):

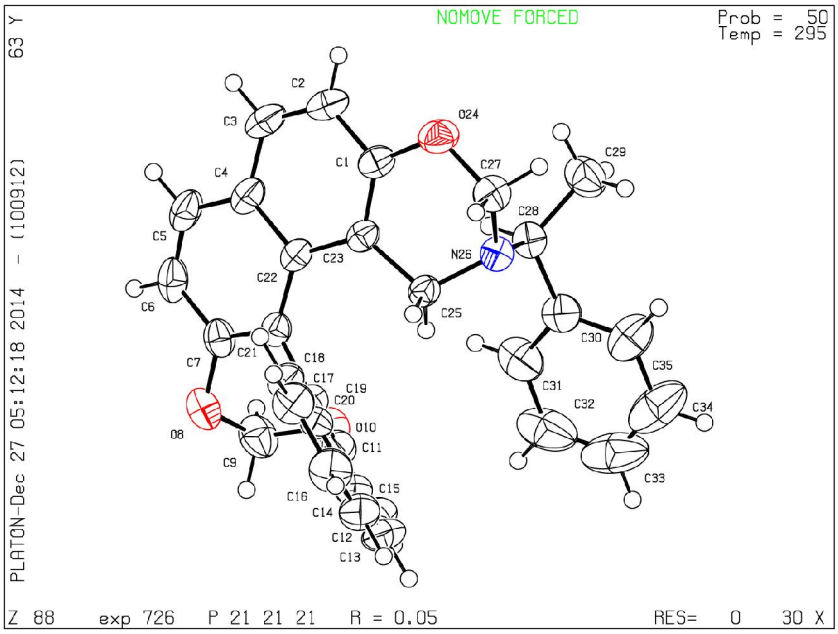


Figure 9: ORTEP diagram of (*P,S*)-**13**. Hydrogens are omitted for clarity with atom numbering scheme (50% probability factor for the thermal ellipsoids).

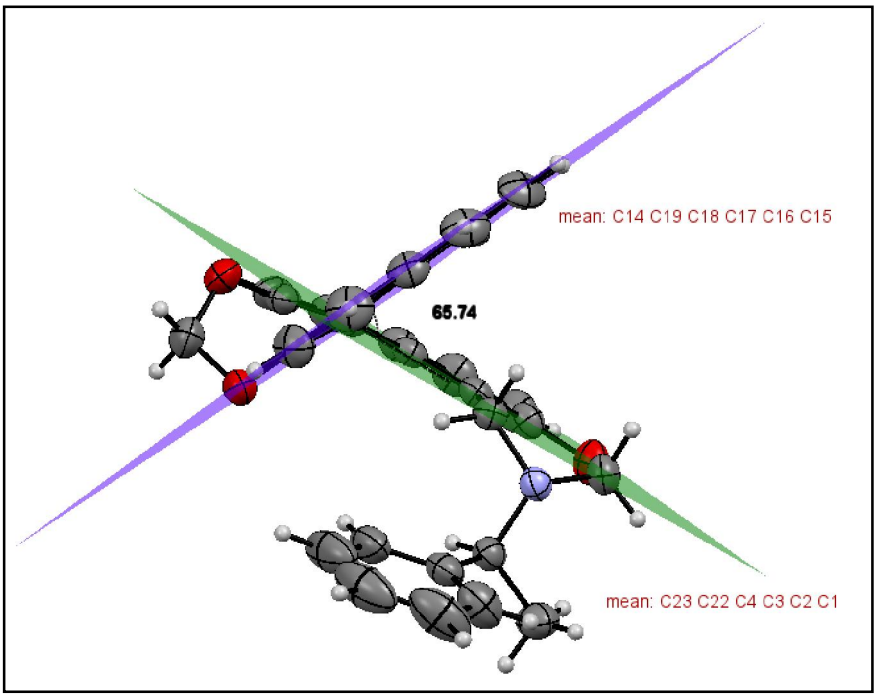


Figure 10: The planes passing through the molecule from the carbons C-14-C19-C18-C17-C16-C15 and C23-C22-C4-C3-C2-C1 showing the twist and the angle between the two planes are 65.74

Table 8 Crystal data and structure refinement for compound (*P,S*)-**13.**

Identification code	exp_726
Empirical formula	$C_{32}H_{24}O_3N_{0.25}$
Formula weight	459.52
Temperature/K	295
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	9.0291(3)
b/Å	12.1317(4)
c/Å	21.5315(9)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2358.53(15)
Z	4
ρ_{calc}g/cm^3	1.2941
μ/mm^{-1}	0.659
F(000)	968.0
Radiation	(λ = 1.54184)
2Θ range for data collection/°	8.22 to 146.82
Index ranges	$-11 \le h \le 6$, $-14 \le k \le 15$, $-25 \le l \le 26$
Reflections collected	8159
Independent reflections	4731 [R_{int} = 0.0333, R_{sigma} = 0.0411]
Data/restraints/parameters	4731/0/332
Goodness-of-fit on F^2	0.807
Final R indexes [I>=2σ (I)]	R_1 = 0.0467
Final R indexes [all data]	R_1 = 0.0520, wR_2 = 0.1346
Largest diff. peak/hole / e Å^{-3}	0.17/-0.28
Flack parameter	-0.1(2)

Table 9 Bond Lengths for compound (*P,S*)-13.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O10	C11	1.385(3)	C19	C14	1.428(3)
O10	C9	1.411(3)	C19	C18	1.419(3)
N26	C25	1.467(2)	C6	C7	1.403(3)
N26	C27	1.409(3)	C6	C5	1.358(4)
N26	C28	1.493(3)	C11	C12	1.408(3)
O24	C1	1.366(3)	C2	C3	1.343(4)
O24	C27	1.466(3)	C29	C28	1.515(3)
O8	C7	1.391(3)	C14	C15	1.414(4)
O8	C9	1.426(3)	C14	C13	1.414(4)
C23	C25	1.523(2)	C28	C30	1.520(3)
C23	C22	1.434(3)	C18	C17	1.372(3)
C23	C1	1.382(3)	C17	C16	1.414(4)
C22	C21	1.443(3)	C30	C31	1.389(4)
C22	C4	1.438(3)	C30	C35	1.389(4)

C1	C2	1.410(3)	C15	C16	1.349(4)
C21	C20	1.498(3)	C31	C32	1.389(4)
C21	C7	1.384(3)	C12	C13	1.362(4)
C4	C3	1.422(3)	C32	C33	1.361(7)
C4	C5	1.413(3)	C35	C34	1.393(5)
C20	C19	1.423(3)	C34	C33	1.389(6)
C20	C11	1.371(3)			

Table10 Bond Angles for compound (*P,S*)-13.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C9	O10	C11	112.48(19)	C20	C11	O10	118.9(2)
C27	N26	C25	108.84(16)	C12	C11	O10	118.8(2)
C28	N26	C25	112.41(15)	C12	C11	C20	122.3(2)
C28	N26	C27	118.29(18)	C3	C2	C1	119.9(2)
C27	O24	C1	115.45(16)	C21	C7	O8	118.9(2)
C9	O8	C7	113.87(18)	C6	C7	O8	117.1(2)
C22	C23	C25	124.49(17)	C6	C7	C21	123.8(2)
C1	C23	C25	116.73(17)	C2	C3	C4	121.0(2)
C1	C23	C22	118.49(17)	C6	C5	C4	121.1(2)
C23	C25	N26	111.19(16)	C15	C14	C19	118.9(2)
C21	C22	C23	124.50(17)	C13	C14	C19	119.5(2)
C4	C22	C23	118.46(19)	C13	C14	C15	121.6(2)
C4	C22	C21	116.95(19)	C29	C28	N26	112.47(18)
C23	C1	O24	124.21(18)	C30	C28	N26	106.98(17)
C2	C1	O24	113.23(19)	C30	C28	C29	113.55(19)
C2	C1	C23	122.5(2)	C17	C18	C19	121.1(2)
C20	C21	C22	126.17(17)	C16	C17	C18	120.4(2)
C7	C21	C22	118.10(18)	C31	C30	C28	120.6(2)
C7	C21	C20	115.69(18)	C35	C30	C28	120.5(2)
C3	C4	C22	119.5(2)	C35	C30	C31	118.8(3)
C5	C4	C22	120.8(2)	C16	C15	C14	122.0(2)
C5	C4	C3	119.5(2)	C32	C31	C30	120.5(4)
C19	C20	C21	123.51(18)	C13	C12	C11	119.6(2)
C11	C20	C21	117.42(19)	C12	C13	C14	120.6(2)
C11	C20	C19	118.86(19)	C15	C16	C17	119.7(2)
C14	C19	C20	118.8(2)	O8	C9	O10	112.66(19)
C18	C19	C20	123.23(19)	C33	C32	C31	120.6(4)
C18	C19	C14	117.9(2)	C34	C35	C30	120.2(3)
O24	C27	N26	113.66(17)	C33	C34	C35	120.1(4)
C5	C6	C7	118.3(2)	C34	C33	C32	119.8(3)