

SYNTHESIS OF CYCLE B FUNCTIONALIZED DERIVATIVES OF (+)-LARIXOL

Alexandru Ciocarlan ^{a*}, Lidia Lungu ^a, Svetlana Blaja ^a, Sergiu Shova ^b, Aculina Aricu ^a

^a Moldova State University, Institute of Chemistry 3, Academiei str., Chisinau MD-2028, Republic of Moldova

^b 'Petru Poni' Institute of Macromolecular Chemistry of the Romanian Academy, 41A, Grigore Ghica Voda Aleea,
Iasi RO-700487, Romania

*e-mail: algciocarlan@yahoo.com

Received: 29 January 2024/ Revised final: 17 April 2024/ Accepted: 23 April 2024

Table S1

Crystallographic data and details of structure refinement for 8.

Parameters	Compound 8
Emp. formula	C ₂₄ H ₃₆ O ₆
Fw	420.53
T [K]	200.00(14)
space group	P2 ₁
a [Å]	6.4066(5)
b [Å]	8.2146(5)
c [Å]	22.0957(13)
α	90
β [°]	90.018(7)
γ	90
V [Å ³]	1162.84(14)
Z	2
ρ _{calcd} [g cm ⁻³]	1.201
μ [mm ⁻¹]	0.085
Crystal size [mm]	0.40×0.10×0.10
2θ range	5.29 to 50.048
Refls. collected	13460
Indep. Refls., R _{int}	4121, 0.0828
Data/rests./params.	4121/4/278
GOF	1.002
R ₁ , wR ₂ (all data)	0.0736, 0.1496
CCDC no.	2312910

Table S2

Selected bond distances (Å) and angles (°) for compound 8.

Atom	Atom	(Å)	Atom	Atom	(Å)
O1	C2	1.370(7)	C6	C17	1.535(8)
O1	C3	1.386(6)	C7	C8	1.579(8)
O2	C2	1.191(7)	C7	C13	1.536(8)
O3	C21	1.460(8)	C7	C14	1.540(8)
O3	C23	1.349(8)	C8	C10	1.566(8)
O4	C23	1.191(9)	C10	C11	1.539(8)

O5	O6	1.474(5)	C10	C15	1.539(8)
O5	C5	1.469(7)	C10	C16	1.542(8)
O6	C8	1.465(7)	C11	C12	1.527(8)
C1	C2	1.485(8)	C12	C13	1.527(8)
C3	C4	1.310(8)	C17	C18	1.536(8)
C3	C8	1.510(8)	C18	C21	1.525(8)
C4	C5	1.490(8)	C19	C20	1.203(11)
C5	C6	1.533(8)	C19	C21	1.513(11)
C5	C9	1.512(8)	C21	C22	1.523(9)
C6	C7	1.585(8)	C23	C24	1.474(12)

Table S3

Bond Angles for compound 8.							
Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	O1	C3	123.1(5)	O6	C8	C7	105.9(4)
C23	O3	C21	122.1(6)	O6	C8	C10	100.8(4)
C5	O5	O6	110.1(4)	C3	C8	C7	107.4(4)
C8	O6	O5	113.0(4)	C3	C8	C10	118.6(5)
O1	C2	C1	109.2(6)	C10	C8	C7	116.1(5)
O2	C2	O1	123.2(6)	C11	C10	C8	108.6(5)
O2	C2	C1	127.6(6)	C11	C10	C16	107.7(5)
O1	C3	C8	115.6(5)	C15	C10	C8	115.0(5)
C4	C3	O1	129.1(5)	C15	C10	C11	108.2(5)
C4	C3	C8	115.3(5)	C15	C10	C16	107.6(5)
C3	C4	C5	113.7(6)	C16	C10	C8	109.4(5)
O5	C5	C4	106.2(5)	C12	C11	C10	113.6(5)
O5	C5	C6	106.3(5)	C13	C12	C11	110.1(5)
O5	C5	C9	101.6(5)	C12	C13	C7	114.1(5)
C4	C5	C6	111.4(5)	C6	C17	C18	113.1(5)
C4	C5	C9	114.2(5)	C21	C18	C17	115.4(5)
C9	C5	C6	115.7(5)	C20	C19	C21	130.0(11)
C5	C6	C7	109.2(5)	O3	C21	C18	103.5(5)
C5	C6	C17	112.8(5)	O3	C21	C19	113.6(6)
C17	C6	C7	116.4(5)	O3	C21	C22	110.0(6)
C8	C7	C6	107.0(4)	C19	C21	C18	110.2(6)
C13	C7	C6	108.1(5)	C19	C21	C22	109.8(7)
C13	C7	C8	108.7(4)	C22	C21	C18	109.6(6)
C13	C7	C14	110.5(5)	O3	C23	C24	110.6(8)
C14	C7	C6	112.1(5)	O4	C23	O3	124.1(8)
C14	C7	C8	110.3(5)	O4	C23	C24	125.3(8)
O6	C8	C3	106.7(5)				

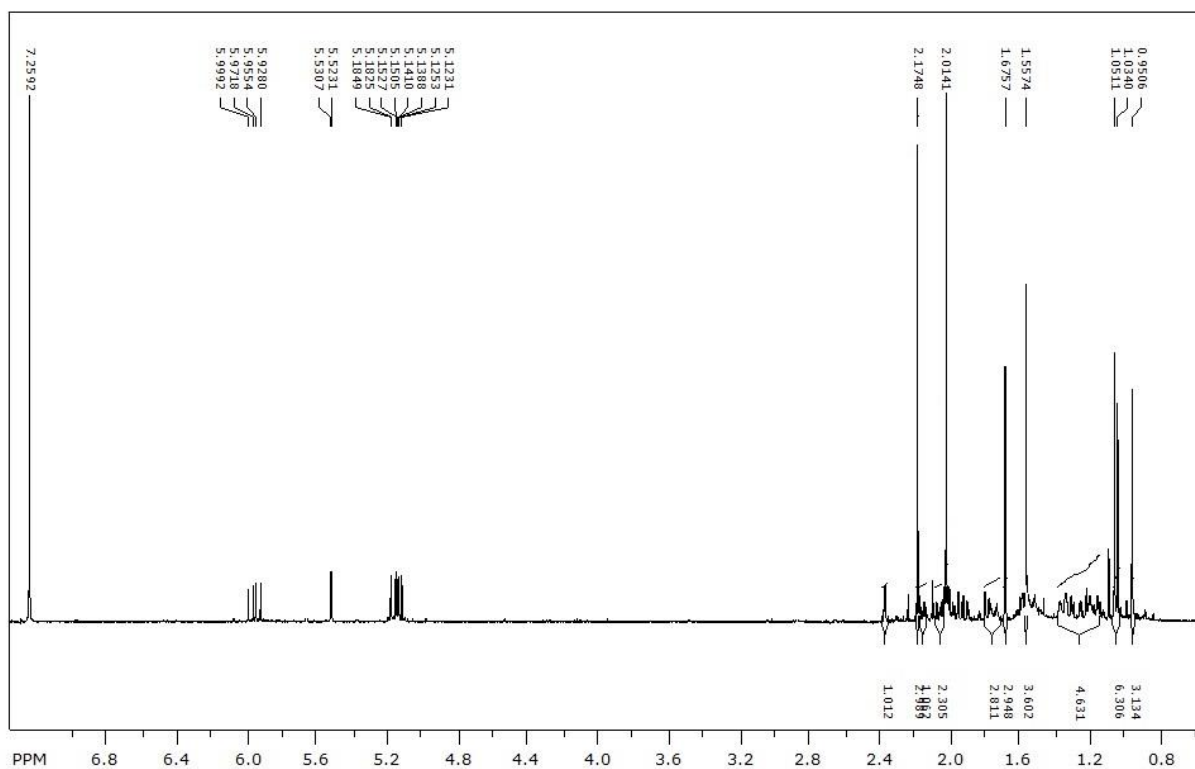


Figure S1. The ^1H NMR spectrum of compound 5.

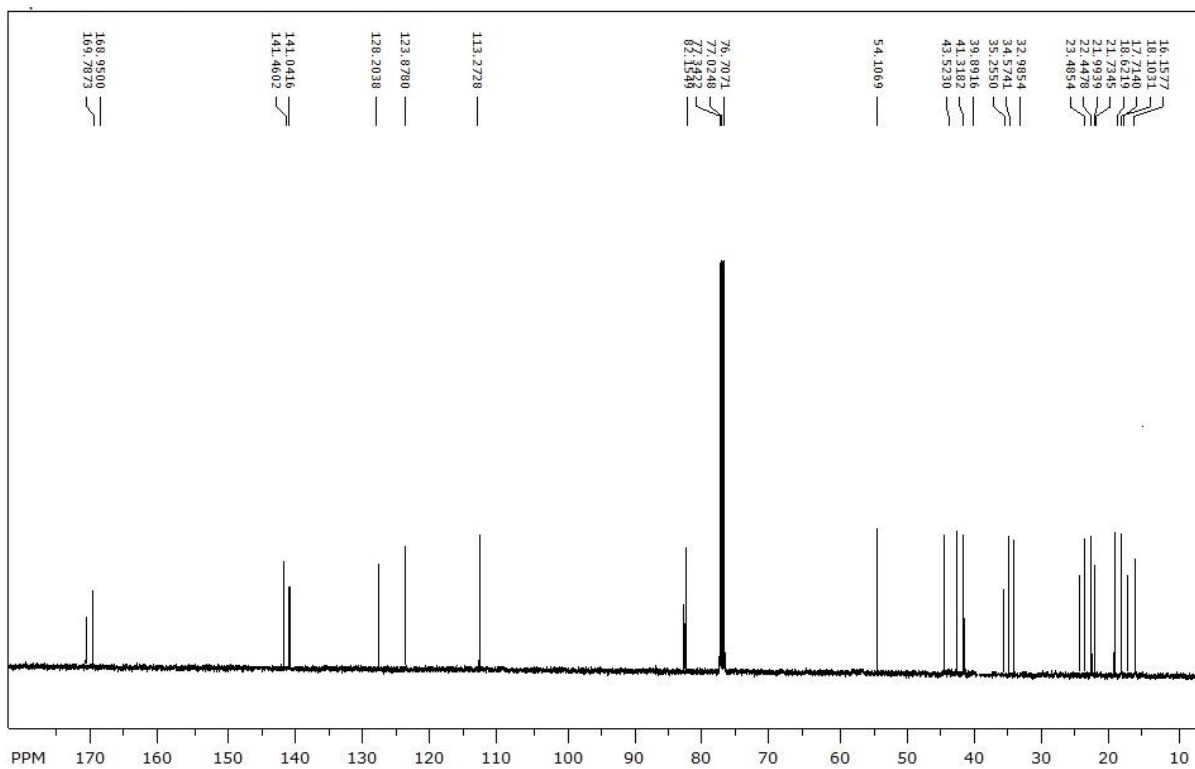


Figure S2. The ^{13}C NMR spectrum of compound 5.

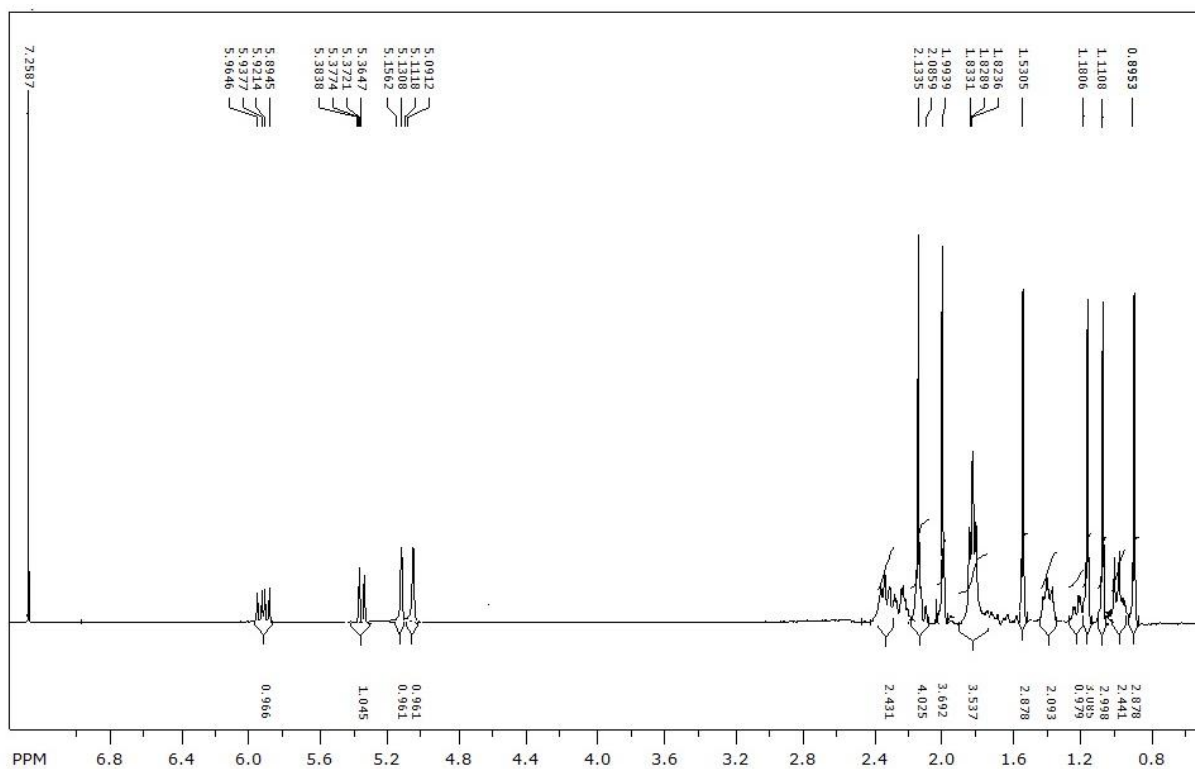


Figure S3. The ¹H NMR spectrum of compound 6.

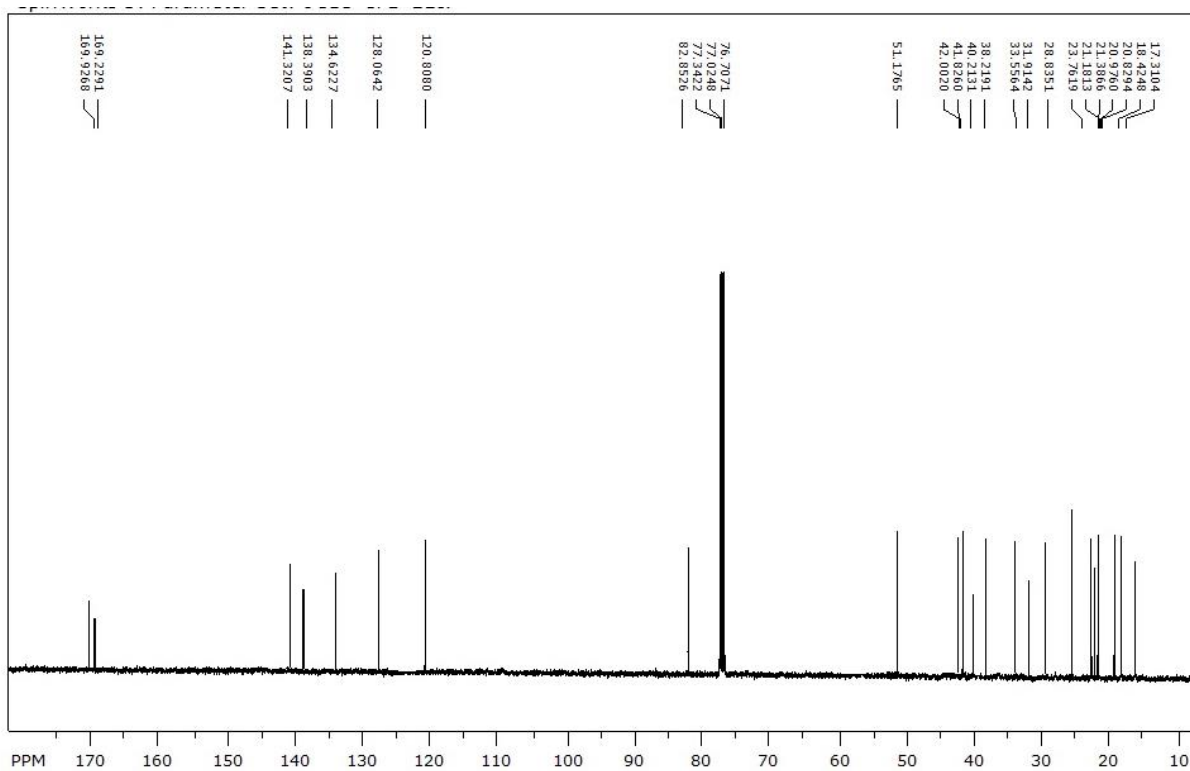
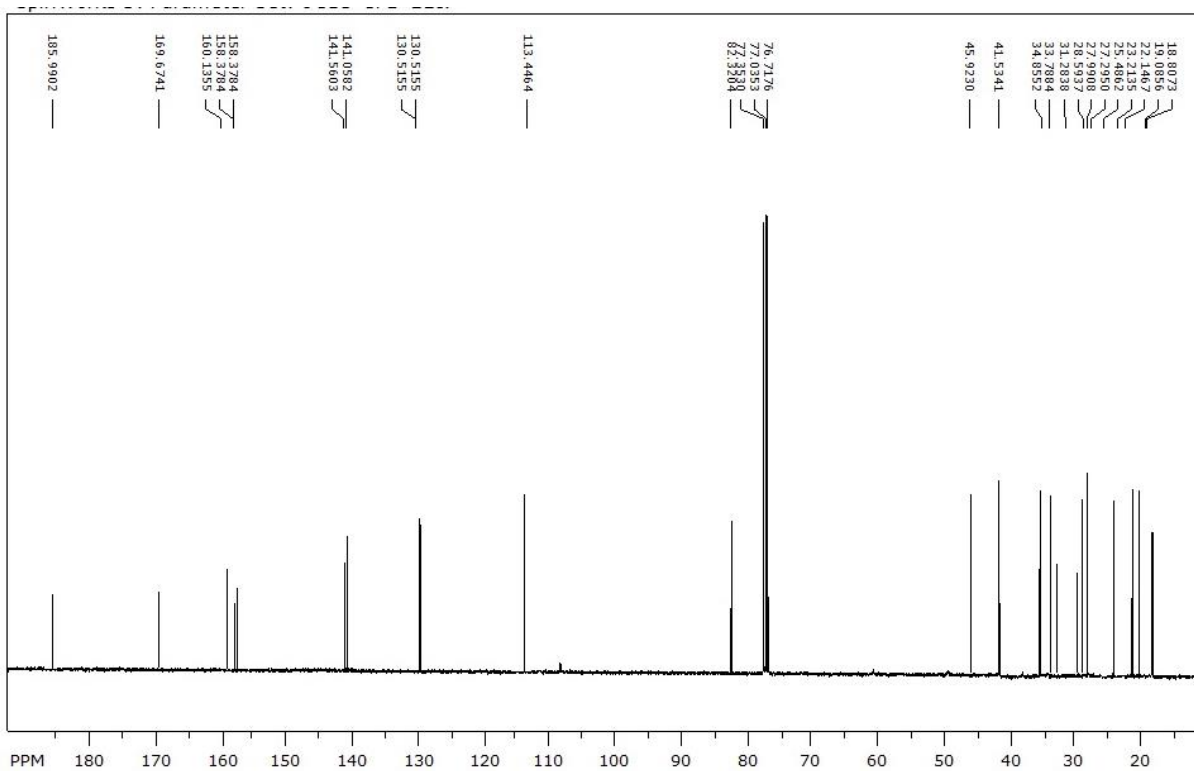
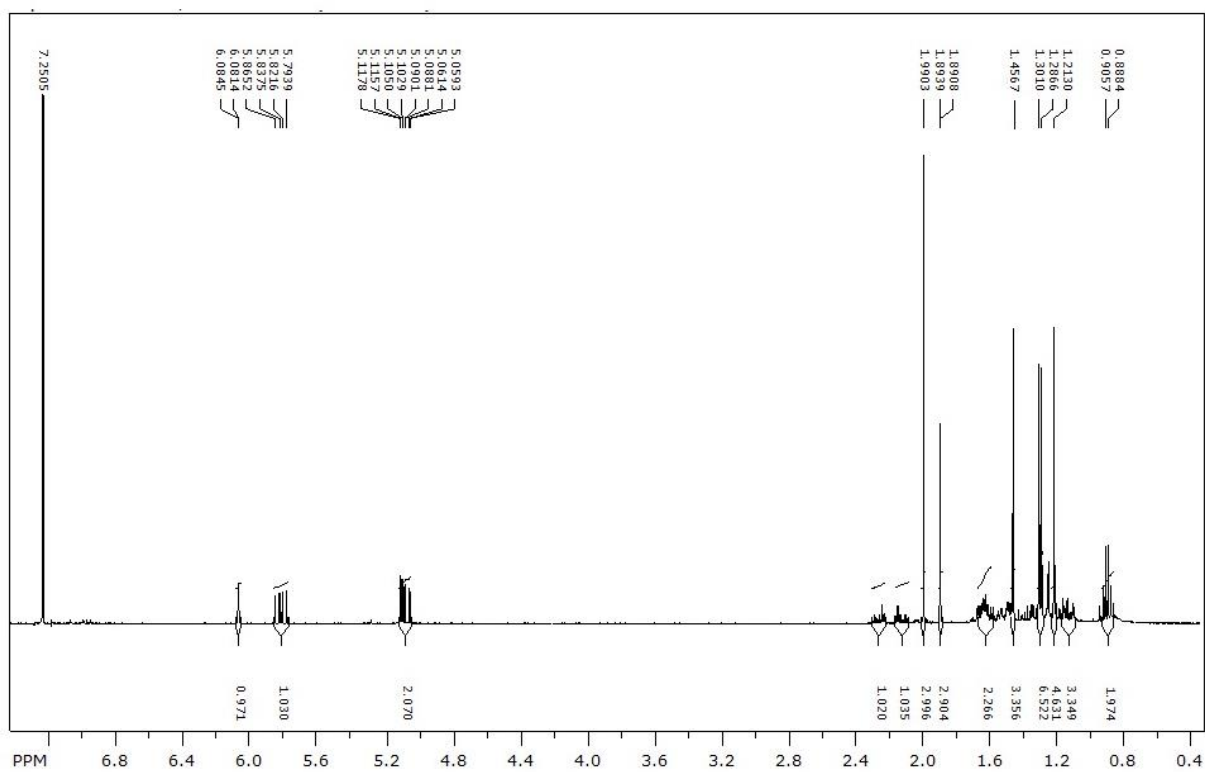


Figure S4. The ¹³C NMR spectrum of compound 6.



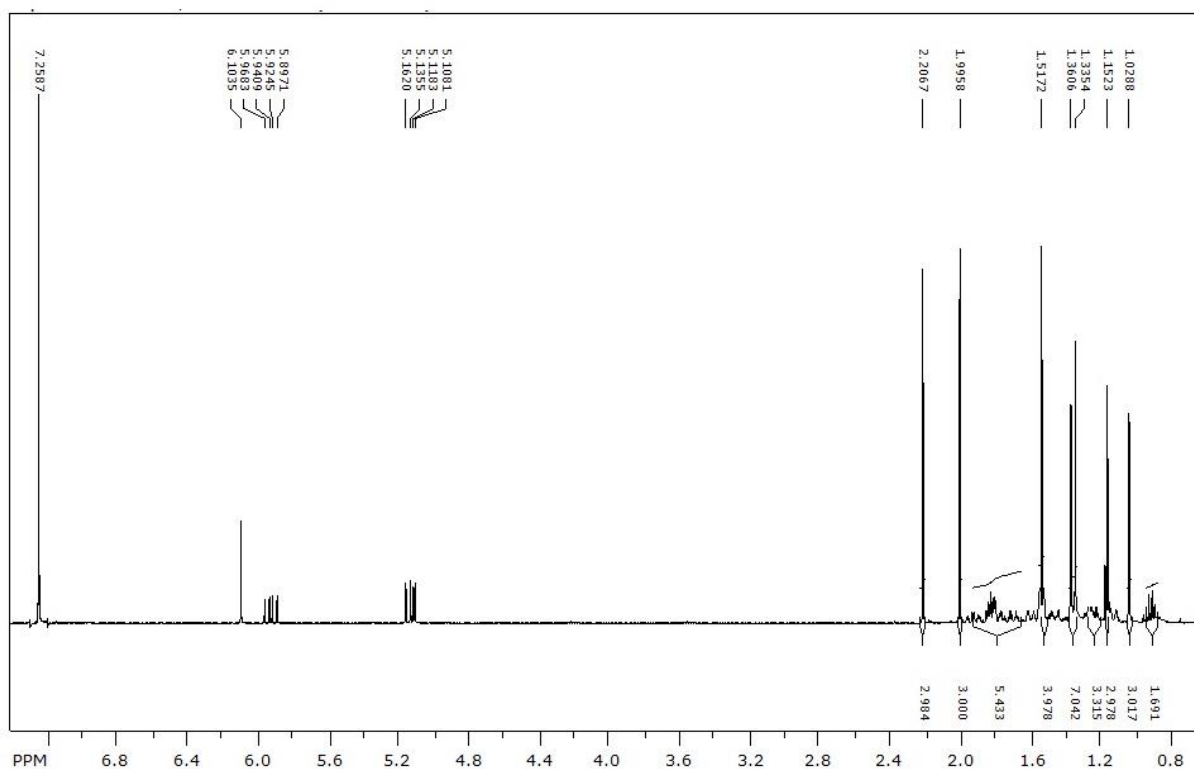


Figure S7. The ^1H NMR spectrum of compound 8.

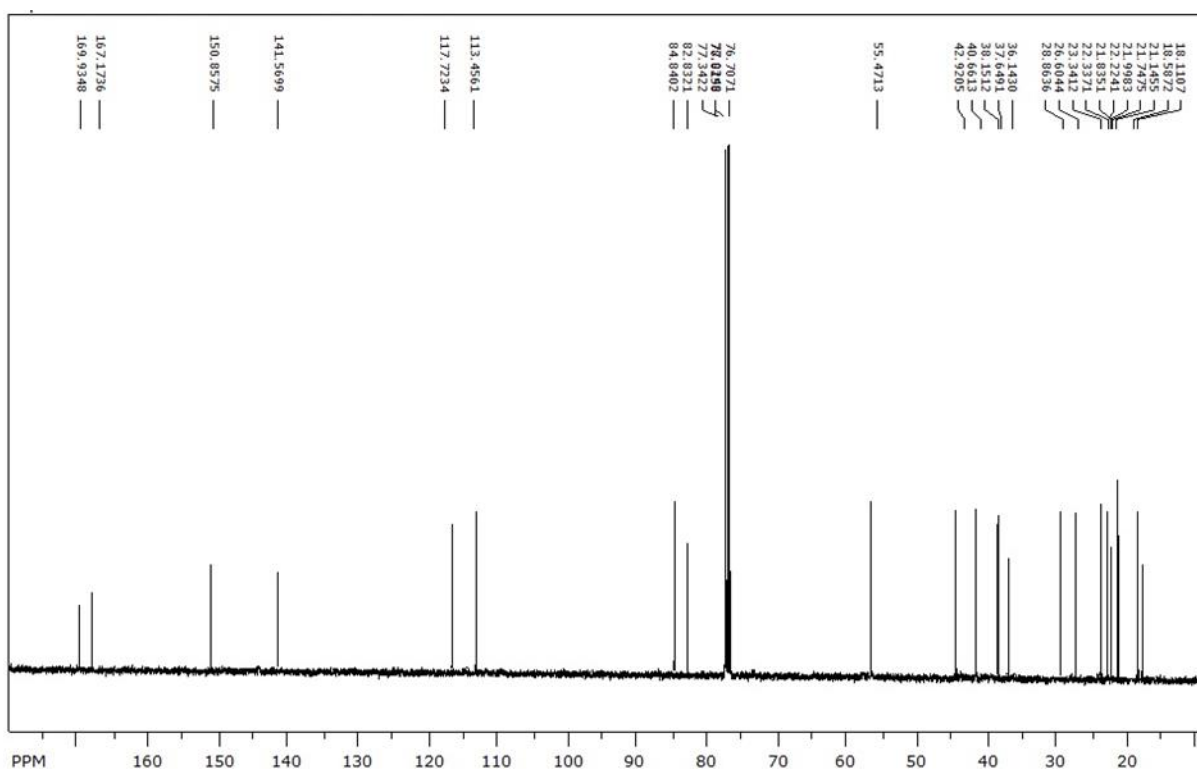


Figure S8. The ^{13}C NMR spectrum of compound 8.