Supporting Information

Microwave-assisted synthesis of new fluorinated coumarin-pyrimidine hybrids as potent anticancer agents, their DNA cleavage and X-ray crystal studies

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Contents:

X-ray crystal data of compound (**1a)**

Table S1 presents crystallographic data and X-ray structure parameters. Measurements were made using Bruker SMART CCD area-detector diffractometer with monochromatic Mo *K*α radiation at room temperature. The crystalline state of a crystal is characterized by a long range, well defined three dimensional orders. Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 ; molecular graphics: ORTEP-3; software used to prepare material for publication: SHELXL97. E-map provided positions for all non H-atoms. The full-matrix least-squares refinement was carried out on F^2 using anisotropic temperature factors for all non H-atoms. The H-atoms were located from DF-maps, and then their positions were refined using a riding model with isotropic thermal parameters taken as 1.2 times temperature factors for their parent-atoms. The ORTEPs of these isomers were obtained by the PLATON program. Coordinates were deposited in the Cambridge Crystallographic Data Centre with deposit number CCDC-897297.

Table-S1: Crystal data, Data collection and Structure refinement of compound (**1a**)

Empirical formula	$C_{27}H_{19}FN_2O_2$
Formula weight	422.44
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic P-1
Unit cell dimensions	a = 8.0072(3)Å b = 10.1043(4)Å c = 13.2110(5)Å α = 100.264(2)°, β= 90.006(2)° γ = 93.327(3)°
Volume	1049.93(7)Å ^{3}
Z	2
Calculated density	1.336mg/m^3
Crystal size	0.22 × 0.15 × 0.12 mm
Absorption coefficient	0.091mm^{-1}
F(000)	440
Crystal form	Prism, colourless
Radiation source	fine-focus sealed tube
Radiation type	Mo *Kα*
Radiation monochromator	graphite
Criterion for observed reflection	I > 2σ(I)
Data collection	
Diffractometer	Bruker SMART CCD area-detector
Data collection method	ω- χ scans
Absorption correction	multi-scan
Theta range for data collection	1.57 to 23.64°
Limiting indices	$-9 \le h \le 8$, $-11 \le k \le 10$, $-14 \le l \le 14$
Reflections collected / unique	3127 / 2458 [R(int) = 0.0200]
Completeness to theta	99.4 %
Max. and min. transmission	T_{max} = 1.000, T_{min} = 0.790
Refinement	
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2458 / 0 / 290
Goodness-of-fit on F^2	1.07
Final R indices [I>2σ(I)]	R1 = 0.0470, wR2 = 0.1375
R indices (all data)	R1 = 0.0593, wR2 = 0.1472
Weighting scheme	$\omega = 1/\left[\sigma^2\left(F_o^2\right) + (0.0714P)^2 + 0.2386P\right]$ $Where\ P = \left(F_o^2 + 2F_c^2\right)/3$
(Δ/σ)max	< 0.001
Largest diff. peak and hole	0.284 and -0.155e.Å^{-3}

Table-S2: Selected equivalent isotropic displacement parameters ($Å^2$) for (**1a)**

	x	y	z	*U*iso*/*U*eq
F1	0.7866(3)	0.1243(2)	0.4 32 (12)	0.1726 (10)
O2	0.93813(17)	0.80366(12)	0.98952(10)	0.0638 (4)
O3	0.80510(19)	0.74700(14)	1.12113(11)	0.0756 (5)
N4	0.5307(2)	0.25470(14)	1.06110(11)	0.0560 (4)
N5	0.7030 (2)	0.35088(14)	0.94376(11)	0.0552(4)
C6	0.8502(2)	0.70883(19)	1.03431(15)	0.0558(5)
C7	0.8210(2)	0.57545(17)	0.97205(13)	0.0465(4)
H8	0.8708	0.4636	0.8388	0.059*

Table-S3: Selected atomic displacement parameter (Å^2) for (**1a**)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F1	0.3 12 (3)	0.1400 (16)	0.0658 (10)	-0.0224 (17)	0.0577 (14)	0.0295 (10)
O2	0.0749 (9)	0.0468 (8)	0.0634 (9)	-0.0121 (6)	0.0109 (7)	-0.0018 (6)
O3	0.0930 (11)	0.0610 (9)	0.0607 (9)	-0.0213 (7)	0.0191 (8)	-0.0133 (7)
N4	0.0769 (11)	0.0421 (9)	0.0468 (9)	-0.0028 (7)	0.0058 (7)	0.0035 (7)
N5	0.0743 (10)	0.03 83(9)	0.0507 (9)	-0.00 14 (7)	0.0065 (7)	0.0034 (7)
C6	0.0562 (11)	0.0516 (11)	0.0554 (12)	-0.0053 (9)	0.0049 (9)	0.0007 (9)
C7	0.0488 (10)	0.0428 (10)	0.0465 (10)	0.0015 (8)	-0.0009 (8)	0.0048 (8)
C8	0.0558 (11)	0.0424 (10)	0.0488 (11)	0.0001 (8)	-0.0005 (8)	0.0049 (8)
C9	0.0484 (10)	0.0495 (11)	0.0523 (11)	0.0019 (8)	-0.0003 (8)	0.0101 (8)
C28	0.0828 (16)	0.0698 (14)	0.0653 (14)	-0.0021 (11)	-0.0027 (11)	0.0026 (11)
C29	0.104 (2)	0.0925 (19)	0.087 (2)	-0.0118 (15)	0.0334 (17)	0.0059 (15)
C30	0.162 (3)	0.0644 (15)	0.0542 (15)	-0.0120 (17)	0.0241 (18)	0.0146 (11)
C31	0.151 (3)	0.0575 (14)	0.0664 (16)	0.0023 (15)	-0.0293 (17)	0.0058 (11)

C32	0.0845 (15)	0.0491 (12)	0.0834 (17)	-0.0056 (10)	-0.0002 (13)	-0.0022 (11)

Table-S4: Selected Bond lengths (Å) and angles (°) for **(1a)**

F1-C30	1.354 (3)	C19-C20	1.384 (3)
O2-C10	1.372 (2)	C19-C24	1.384 (2)
O2-C6	1.374 (2)	C20-C21	1.374 (3)
O3-C6	1.206 (2)	C20-H20	0.93
N4-C16	1.331 (2)	C21-C22	1.382 (3)
N4-C17	1.338 (2)	C21-H21	0.93
N5-C16	1.327 (2)	C22-C23	1.380 (3)
C6-C7	1.455 (2)	C23-C24	1.378 (3)
C7-C8	1.347 (2)	C23-H23	0.93
C8-C9	1.421 (2)	C25-H25A	0.96
C10-O2-C6	123.48 (14)	C21-C20-C19	121.50 (17)
C16-N4-C17	116.89 (15)	C21-C20-H20	119.2
C16-N5-C15	116.87 (15)	C19-C20-H20	119.2
O3-C6-O2	115.55 (16)	C20-C21-C22	121.24 (18)
O2-C10-C11	118.37 (17)	C22-C25-H25A	109.5
O2-C10-C9	120.07 (16)	C22-C25-H25B	109.5
N5-C16-N4	126.41 (15)	C30-C29-C28	118.5 (3)
N5-C16-C26	117.91 (16)	C30-C29-H29	120.7
N4-C16-C26	115.66 (16)	C28-C29-H29	120.7
N4-C17-C18	120.54 (15)	C31-C30-C29	122.3 (2)
N4-C17-C19	116.40 (15)	C31-C30-F1	118.8 (3)
C28-C29-C30-F1	-178.9 (2)	C28-C27-C32-C31	0.7 (3)
C29-C30-C31-C32	-1.3 (4)	C26-C27-C32-C31	-178.91 (17)
F1-C30-C31-C32	178.78 (19)	C30-C31-C32-C27	0.3 (3)

C31-C30-F1	118.8 (3)	C29-C30-F1	118.9 (3)

X-ray crystal data of compound **(1b)**

Table S5 presents crystallographic data and X-ray structure parameters. Measurements were made using Bruker SMART CCD area-detector diffractometer with monochromatic Mo *K*α radiation at room temperature. The crystalline state of a crystal is characterized by a long range, well defined three dimensional orders. E-map provided positions for all non H-atoms. The full-matrix least-squares refinement was carried out on F^2 using anisotropic temperature factors for all non H-atoms. The H-atoms were located from DF-maps, and then their positions were refined using a riding model with isotropic thermal parameters taken as 1.2 times temperature factors for their parent-atoms. The ORTEPs of these isomers were obtained by the PLATON program. Coordinates were deposited in the Cambridge Crystallographic Data center with deposit number. CCDC-897298

Table-S5: Crystal data, Data collection and Structure refinement of compound (**1b**)

Empirical formula	$C_{27}H_{19}FN_2O_3$
Formula weight	438.44

Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic P-1
Unit cell dimensions	a = 8.1330(2)Å b = 10.2945(2)Å c = 12.7544(3)Å α = 101.192(1)°, β= 90.344(1)° γ = 95.499(1)°
Volume	1042.40(4)Å ^{3}
Z	2
Calculated density	1.397mg/m^3
Crystal size	0.22 × 0.15 × 0.12 mm
Absorption coefficient	0.098mm^{-1}
F(000)	456
Crystal form	Prism, colourless
Radiation source	fine-focus sealed tube
Radiation type	Mo *Kα*
Radiation monochromator	graphite
Criterion for observed reflection	I > 2σ(I)
Data collection	
Diffractometer	Bruker SMART CCD area-detector
Data collection method	ω- χ scans
Absorption correction	multi-scan
Theta range for data collection	1.63to 24.99°
Limiting indices	$-9 \le h \le 9$, $-12 \le k \le 12$, $-15 \le l \le 15$
Reflections collected / unique	17307 / 3656 [R(int) = 0.0210]
Completeness to theta	99.8 %
Max. and min. transmission	T_{max} = 1.000, T_{min} = 0.790
Refinement	
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3656 / 0 / 298
Goodness-of-fit on F^2	1.078
Final R indices [I>2σ(I)]	R1 = 0.0382, wR2 = 0.1056
R indices (all data)	R1 = 0.0469, wR2 = 0.1119
Weighting scheme	$\omega = 1/\left[\sigma^2\left(F_o^2\right) + (0.0714P)^2 + 0.2386P\right]$ $Where\ P = \left(F_o^2 + 2F_c^2\right)/3$
(Δ/σ)max	< 0.001
Largest diff. peak and hole	0.123 and -0.186e.Å^{-3}

Table-S6: Selected equivalent isotropic displacement parameters ($Å^2$) for (**1b**)

x	y	z	*U*iso*/*U*eq

F1	0.29852 (16)	0.57836 (12)	-0.51580 (7)	0.1023
O2	0.44489 (13)	1.30511 (9)	-0.00621 (8)	0.0581
O3	0.30648 (15)	1.25194 (10)	0.12785 (8)	0.0740
O4	-0.28759 (16)	0.91129 (11)	0.52642 (9)	0.0790
N5	0.02512 (15)	0.76412 (11)	0.06938 (8)	0.0519
N6	0.19990 (14)	0.85324 (10)	-0.05386 (8)	0.0501
C7	0.35284 (17)	1.21221 (14)	0.03901 (11)	0.0520
C8	0.32221 (15)	1.07790 (12)	-0.02585 (10)	0.0440
C9	0.38842 (16)	1.05192 (13)	-0.12347 (10)	0.0471(3)
H9	0.3698	0.9662	-0.164	0.056*

Table-S7: Selected atomic displacement parameter ($Å^2$) for **(1b)**

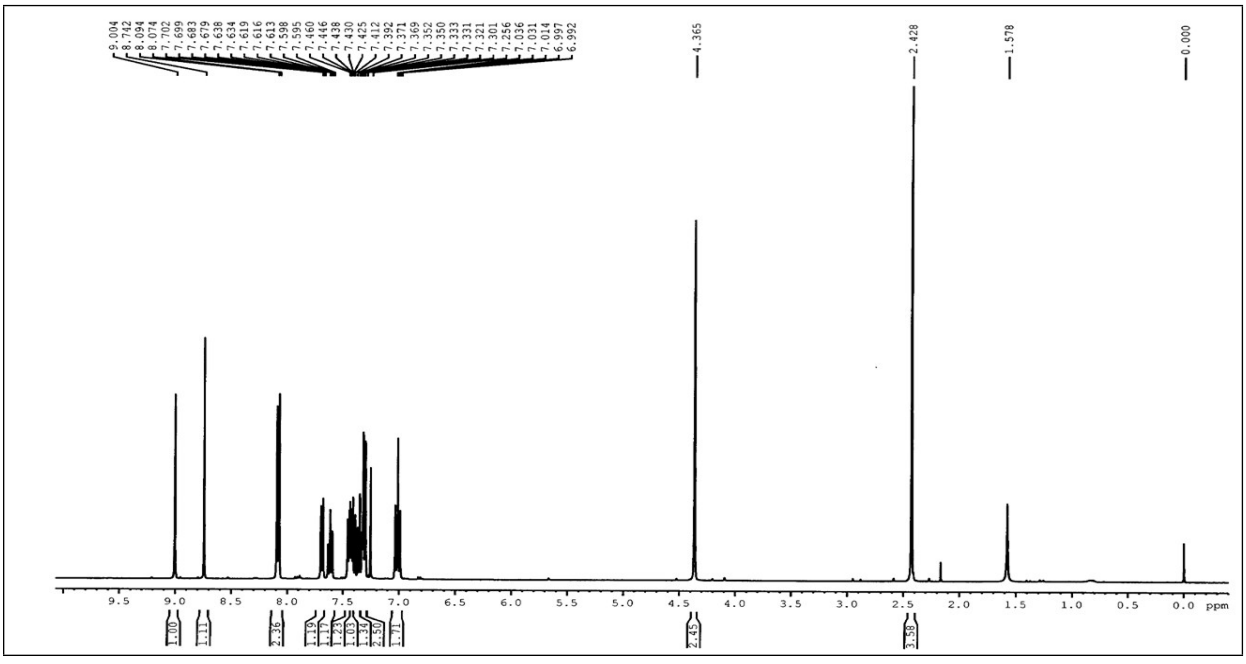
	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F1	0.1393 (10)	0.1083 (9)	0.0555 (6)	-0.0045 (7)	0.0328 (6)	0.0139 (5)
O2	0.0680 (6)	0.0445 (5)	0.0560 (6)	-0.0046 (4)	0.0127 (5)	-0.0002 (4)
O3	0.0925 (8)	0.0577 (6)	0.0586 (6)	-0.0151 (6)	0.0261 (6)	-0.0108 (5)
O4	0.1016 (9)	0.0683 (7)	0.0634 (7)	-0.0029 (6)	0.0354 (6)	0.0083 (5)
N5	0.0658 (7)	0.0432 (6)	0.0449 (6)	0.00 14 (5)	0.0057 (5)	0.0061 (5)
N6	0.0624 (7)	0.0403 (6)	0.0458 (6)	0.0033 (5)	0.0053 (5)	0.0051 (5)
C7	0.0529 (8)	0.0476 (7)	0.0519 (8)	-0.0011 (6)	0.0077 (6)	0.0039 (6)
C8	0.0453 (7)	0.0419 (7)	0.0440 (7)	0.0058 (5)	-0.0006 (5)	0.0057 (5)
C9	0.0525 (7)	0.0419 (7)	0.0461 (7)	0.0072 (6)	0.0006 (6)	0.0054 (5)

C10	0.0457 (7)	0.0467 (7)	0.0473 (7)	0.0084 (6)	0.0022 (5)	0.0096 (6)
C11	0.0479 (7)	0.0506 (7)	0.0491 (7)	0.0059 (6)	0.0039 (6)	0.0087 (6)
C12	0.0662 (9)	0.05 14(8)	0.0673 (9)	-0.0026 (7)	0.0050 (7)	0.0128 (7)
C13	0.0679 (10)	0.0685 (10)	0.0677 (10)	-0.0018 (8)	0.0088 (8)	0.0270 (8)
C14	0.0673 (9)	0.0781 (11)	0.0546 (9)	0.0081 (8)	0.0127 (7)	0.0208 (8)

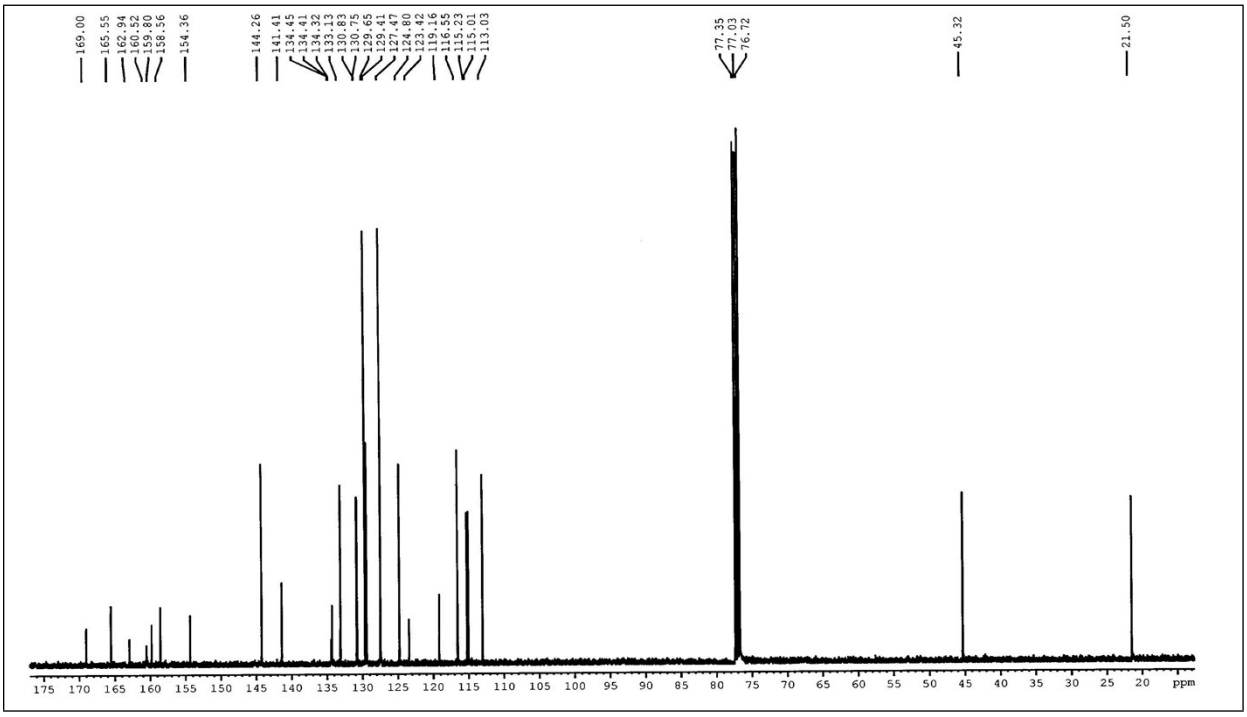
Table-S8: Selected Bond lengths (*Å*) and angles (°) for **(1b)**

F1-C24	1.3615 (16)	C18-C27	1.4757 (17)
O2-C11	1.3743 (16)	C19-H19	0.93
O2-C7	1.3748 (17)	C20-C21	1.5043 (18)
O3-C7	1.2033 (16)	C20-H20A	0.97
O4-C30	1.3647 (16)	C20-H20B	0.97
O4-C33	1.417 (2)	C21-C26	1.375 (2)
N5-C17	1.3378 (16)	C21-C22	1.380 (2)
N5-C18	1.3377 (16)	C22-C23	1.376 (2)
N6-C17	1.3249 (17)	C22-H22	0.93
C11-O2-C7	123.61 (10)	C21-C20-H20B	108.2
C30-O4-C33	117.65 (13)	C17-C20-H20B	108.2
C25VC24VF1	118.72 (16)	C17-N6-C16	116.65 (11)
O3-C7-O2	115.43 (12)	C26-C21-C20	120.97 (15)
N5-C17-C20	114.21 (11)	C31-C32-C27	121.17 (13)

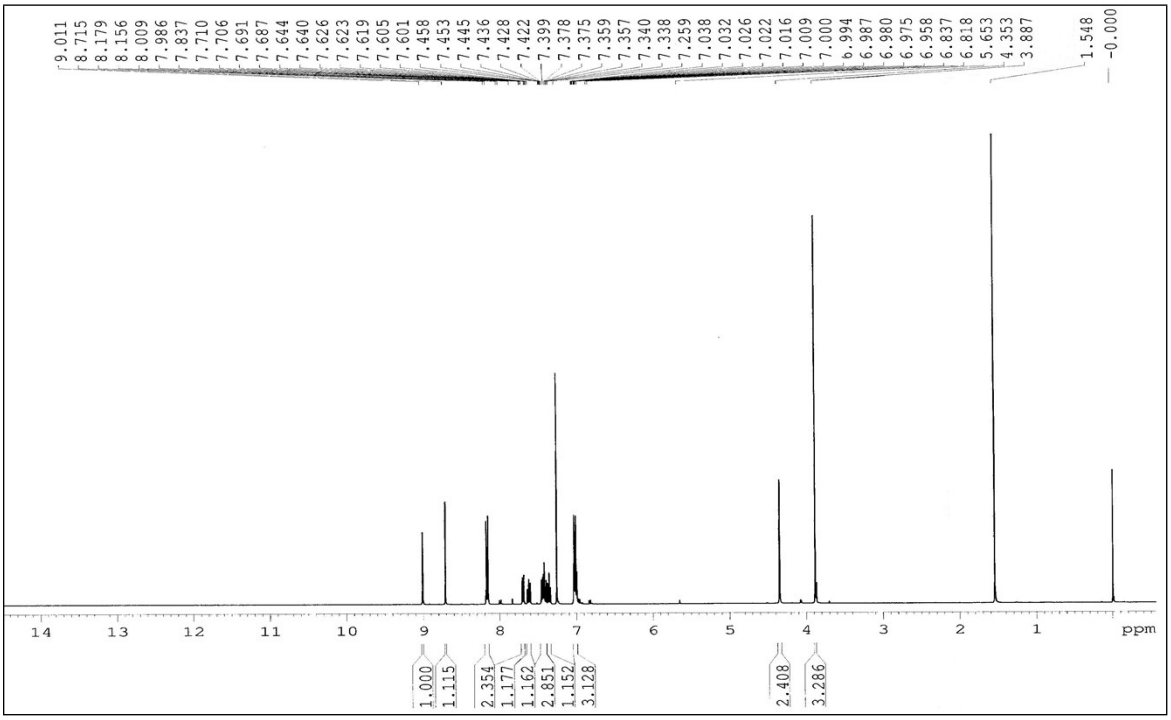
^{1}H NMR spectrum of compound (1a)



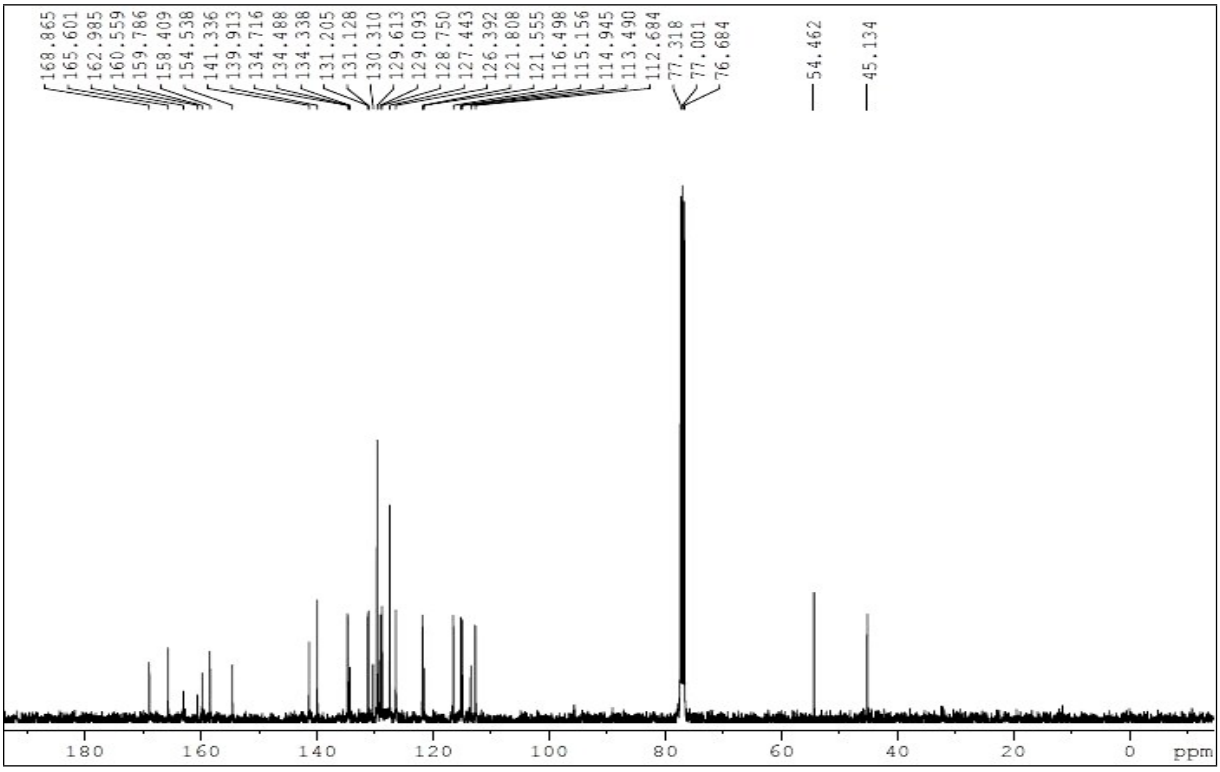
^{13}C NMR spectrum of compound (1a)



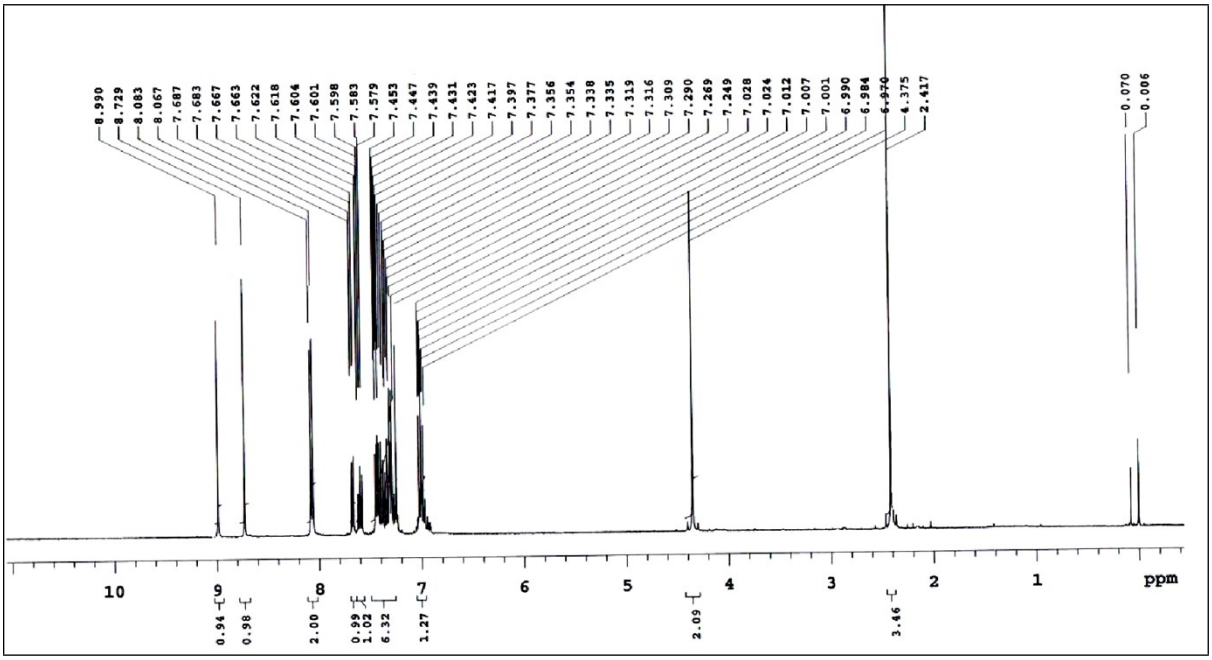
^{1}H NMR spectrum of compound (1b)



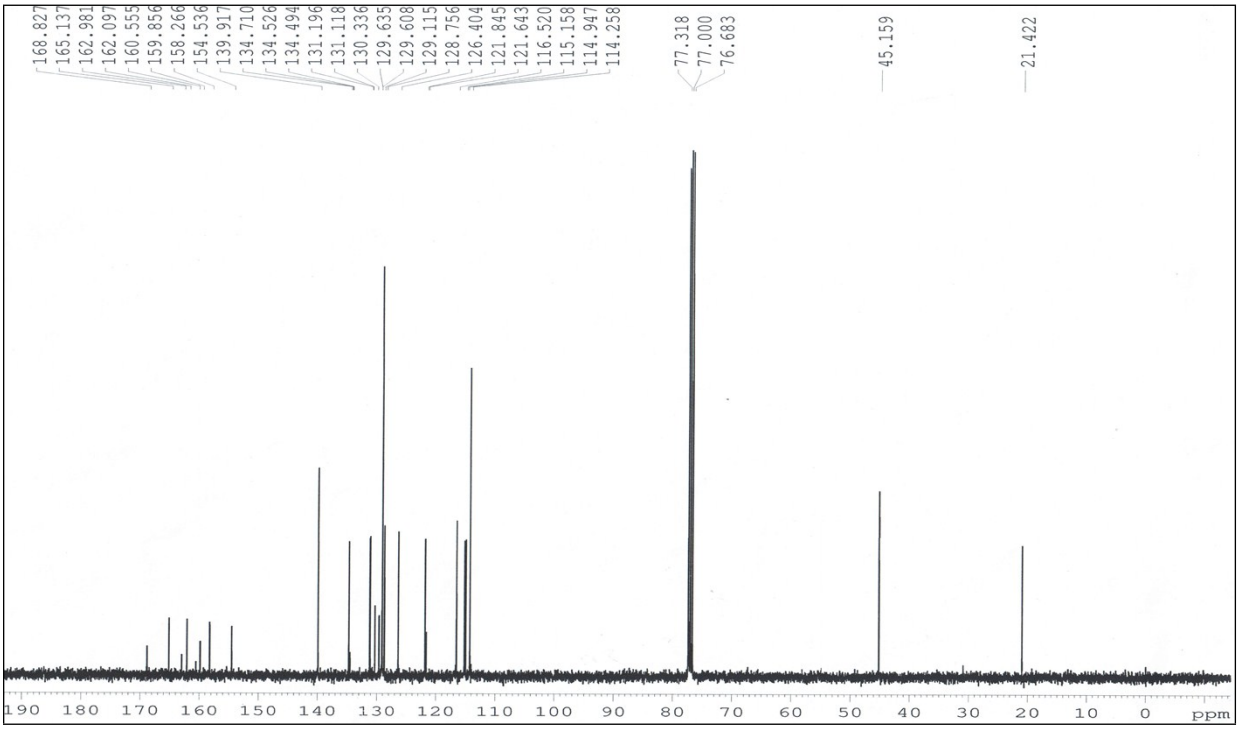
^{13}C NMR spectrum of compound (1b)



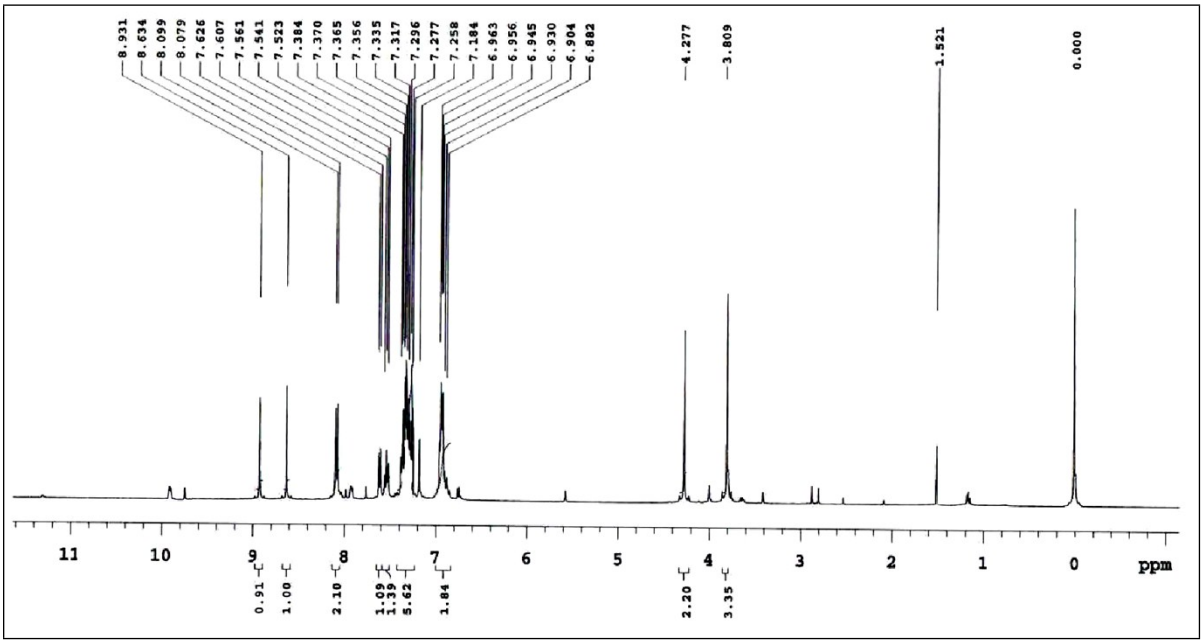
^{1}H NMR spectrum of compound (1c)



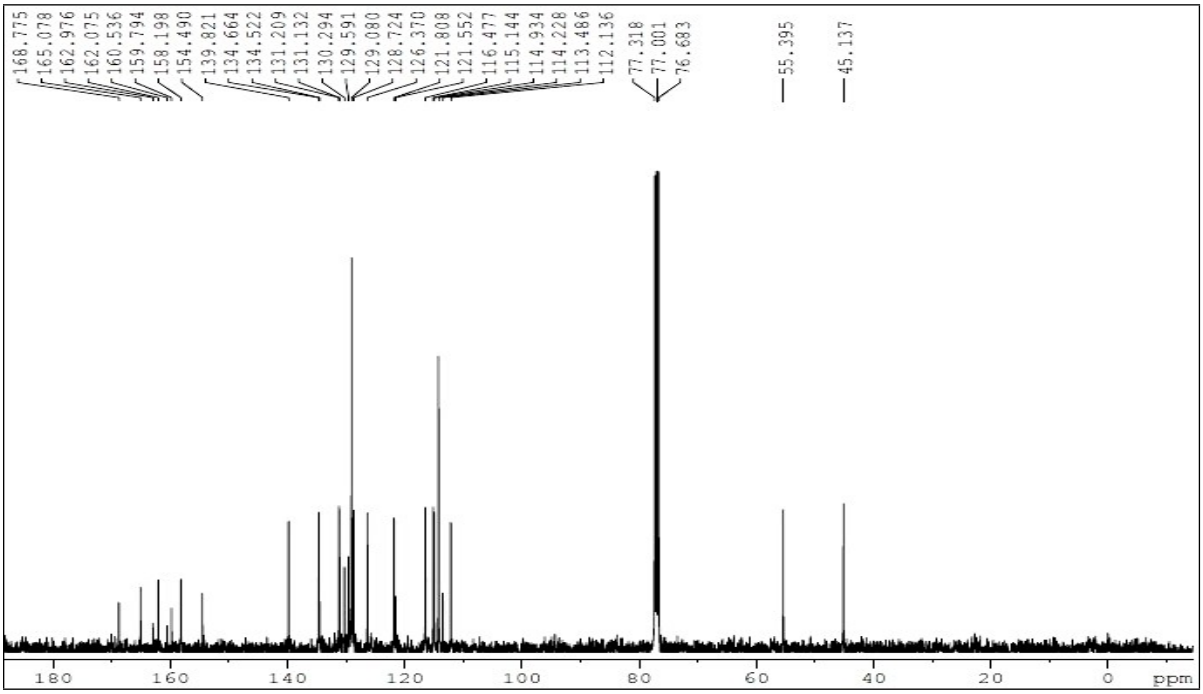
^{13}C NMR spectrum of compound (1c)



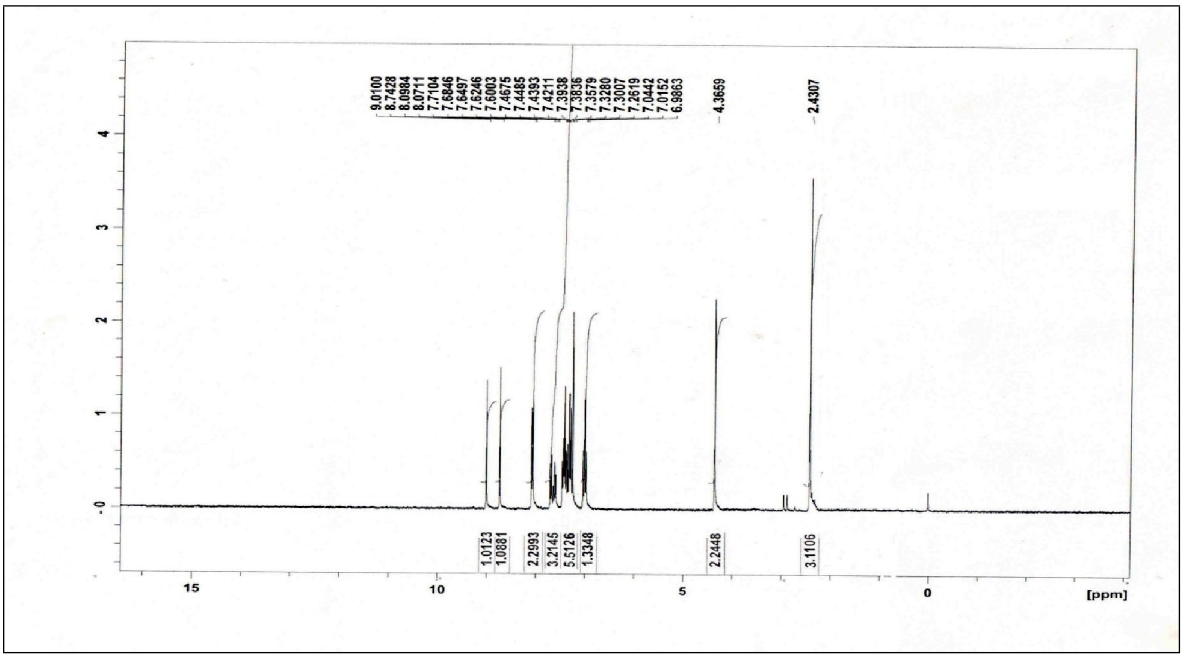
^{1}H NMR spectrum of compound (1d)



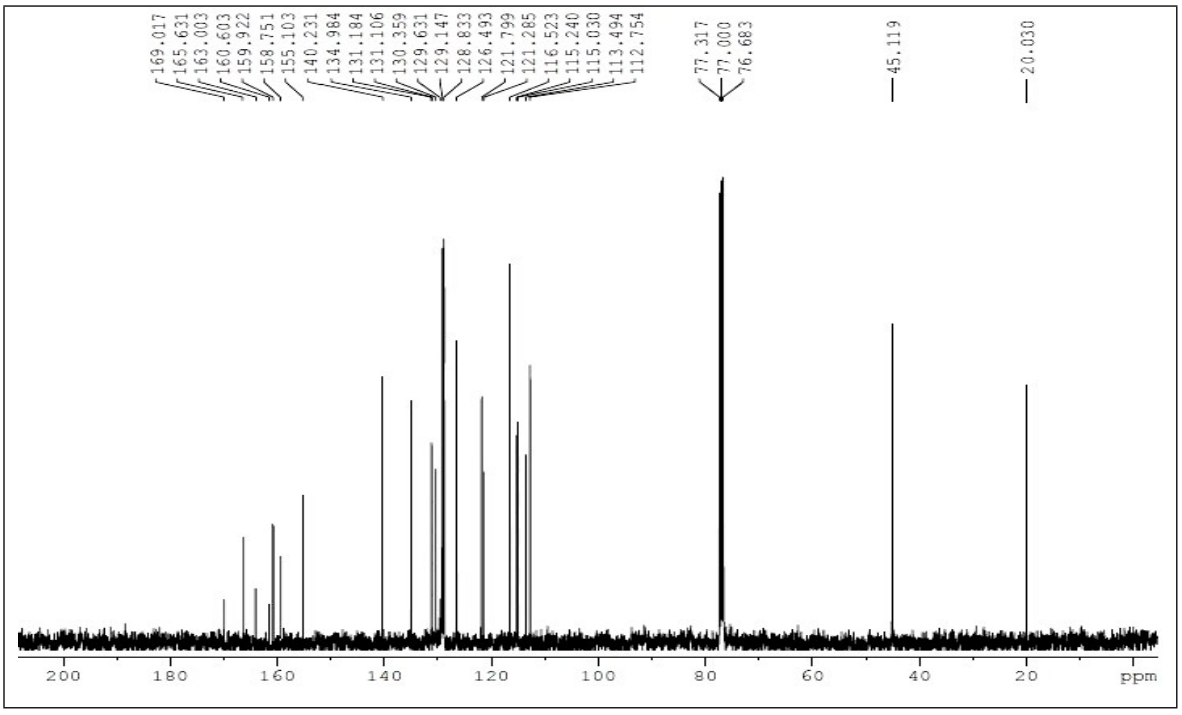
^{13}C NMR spectrum of compound (1d)



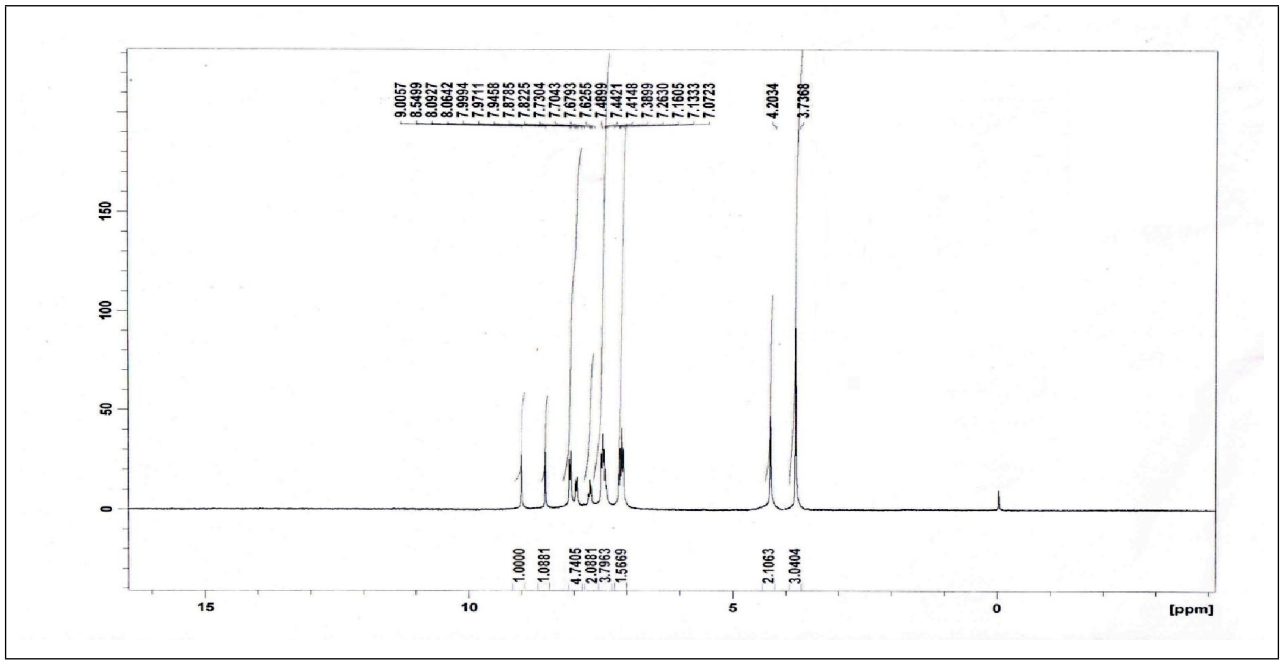
^{1}H NMR spectrum of compound (1e)



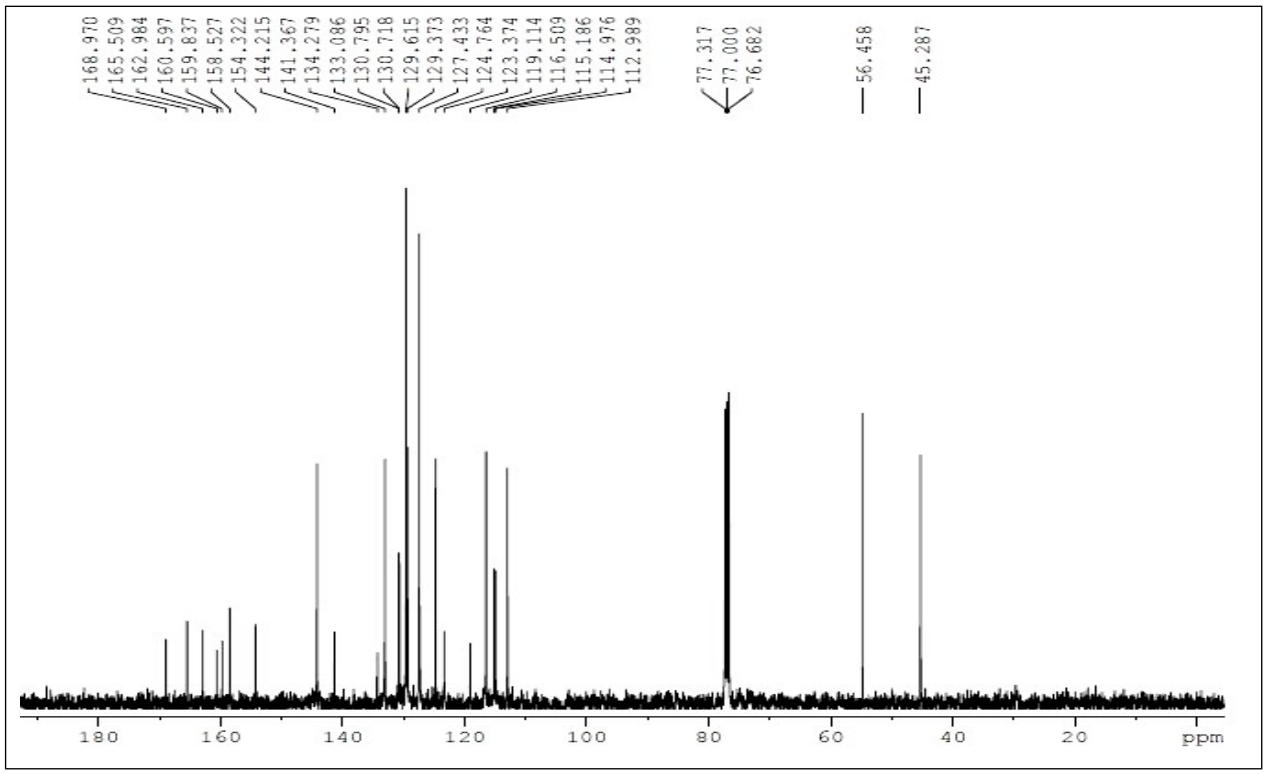
^{13}C NMR spectrum of compound (1e)



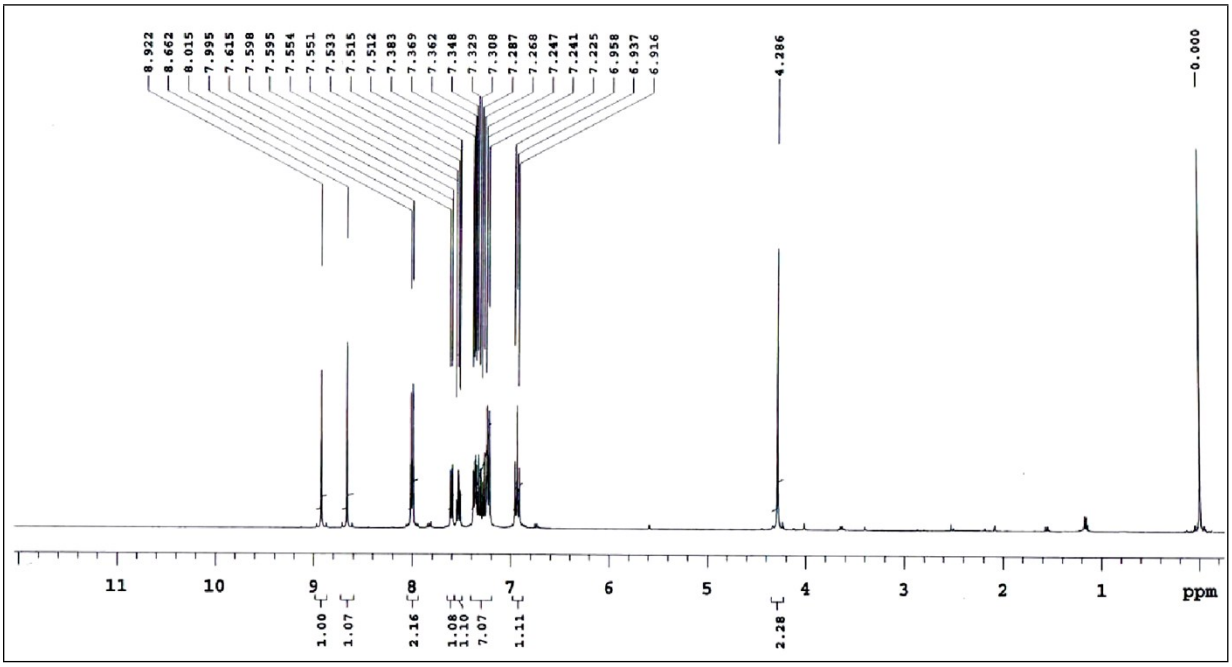
^{1}H NMR spectrum of compound (1f)



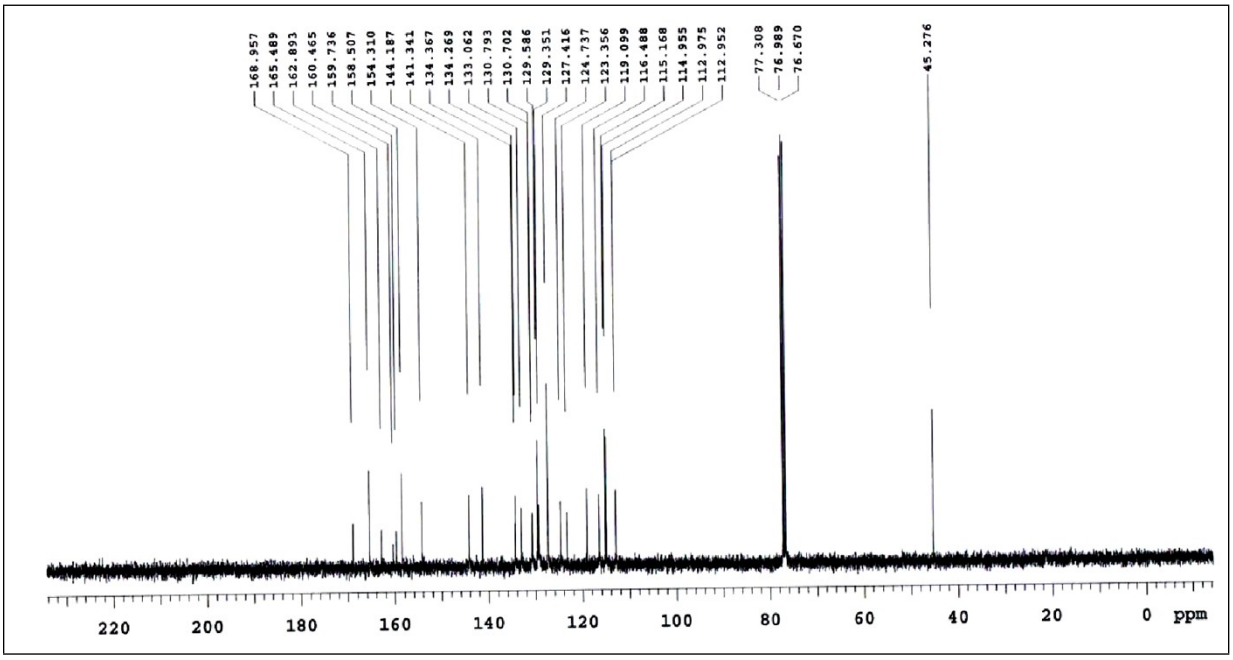
^{13}C NMR spectrum of compound (1f)



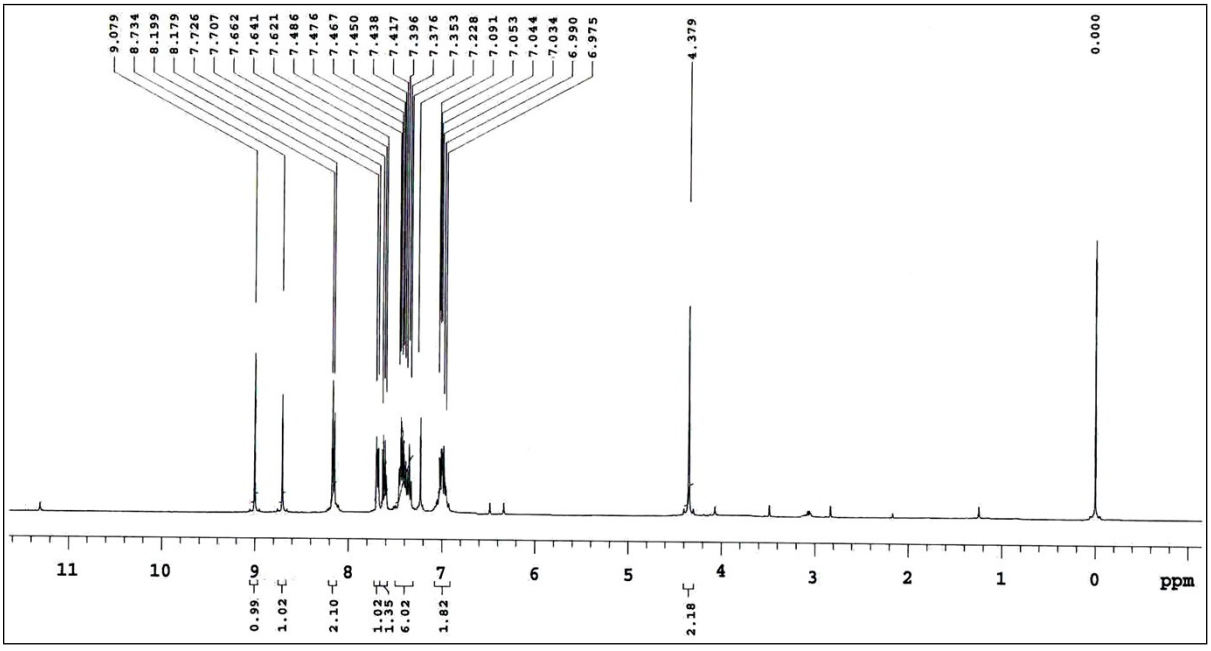
^{1}H NMR spectrum of compound (1g)



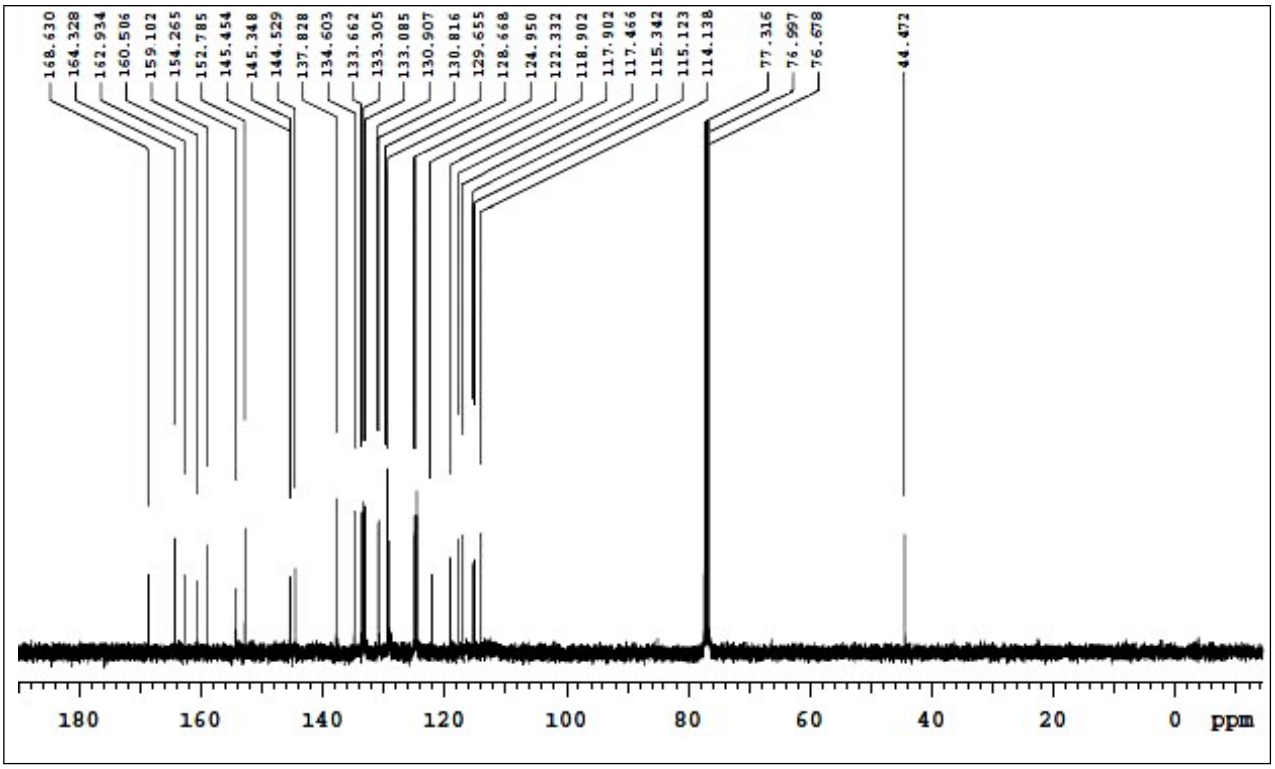
^{13}C NMR spectrum of compound (1g)



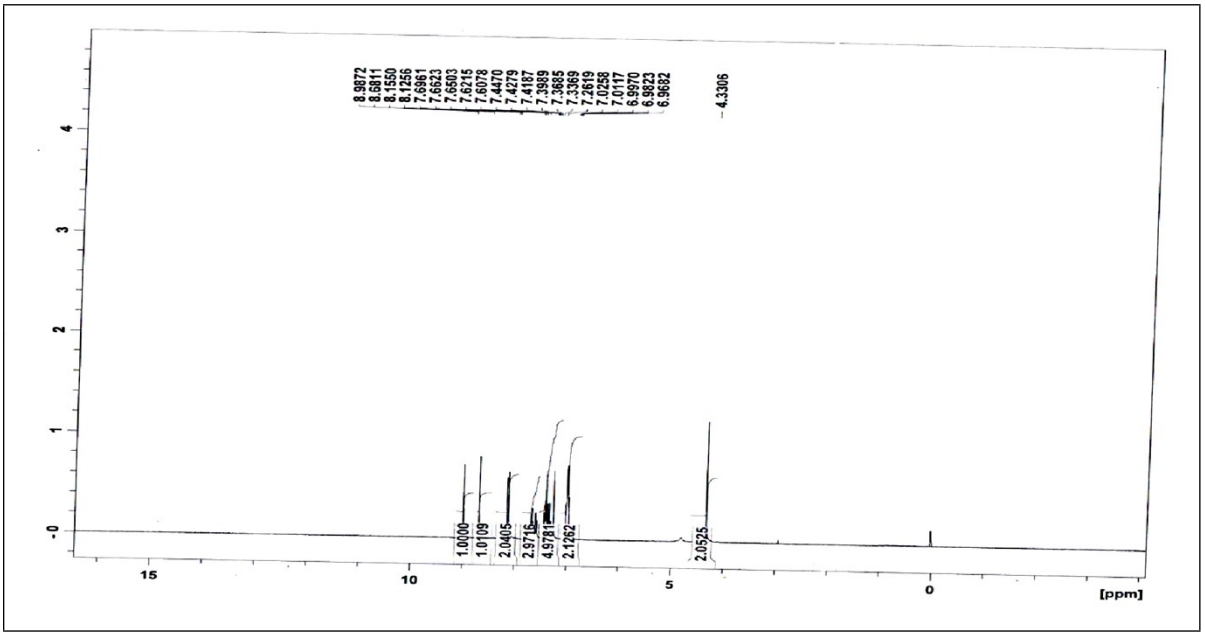
^{1}H NMR spectrum of compound (1h)



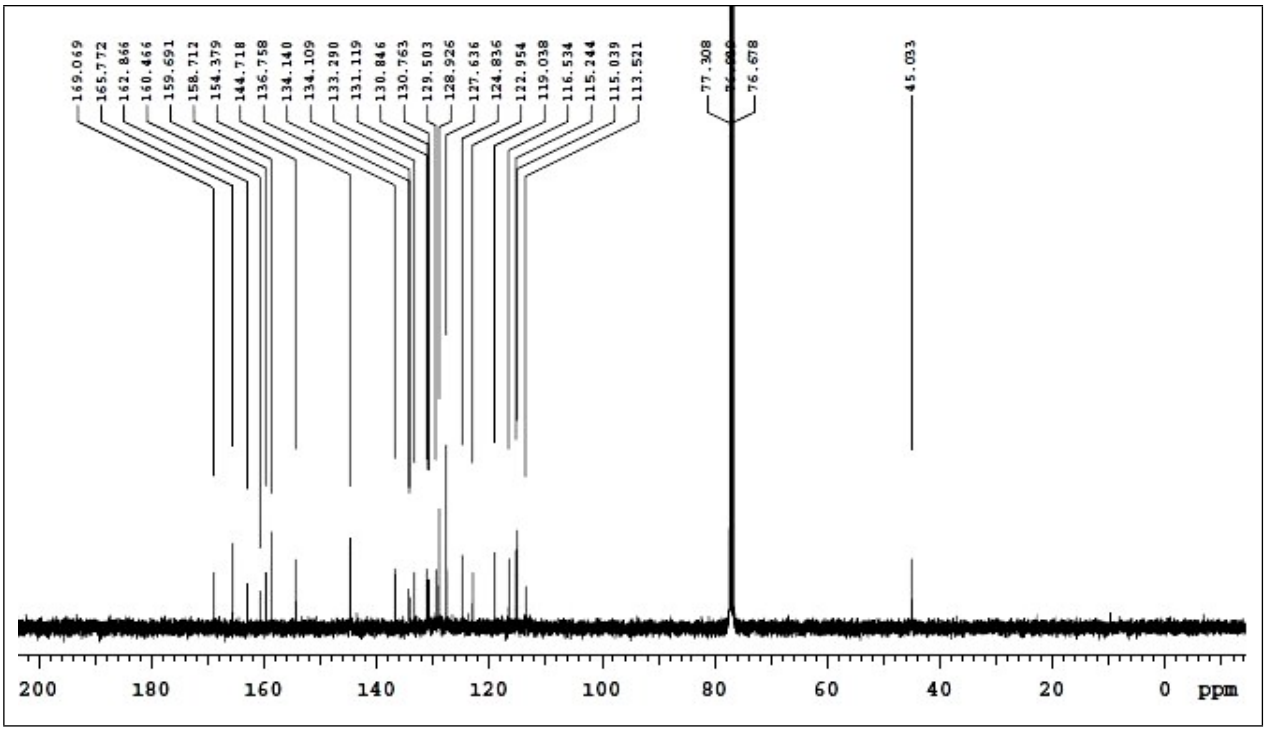
^{13}C NMR spectrum of compound (1h)



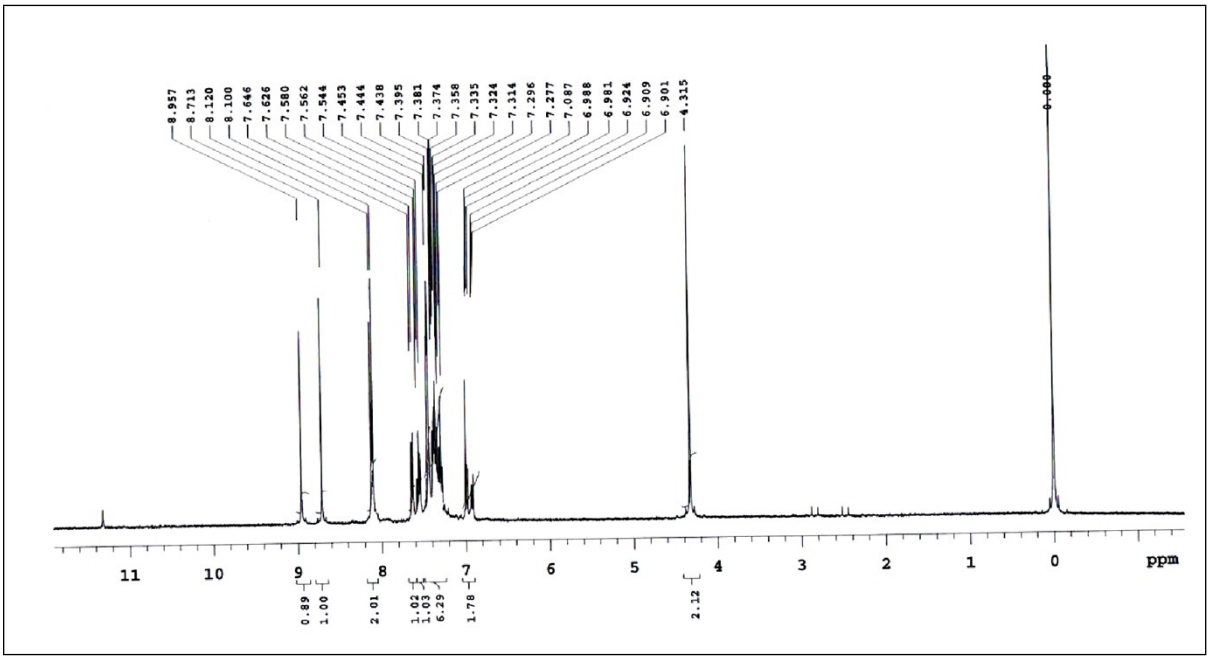
^{1}H NMR spectrum of compound (1i)



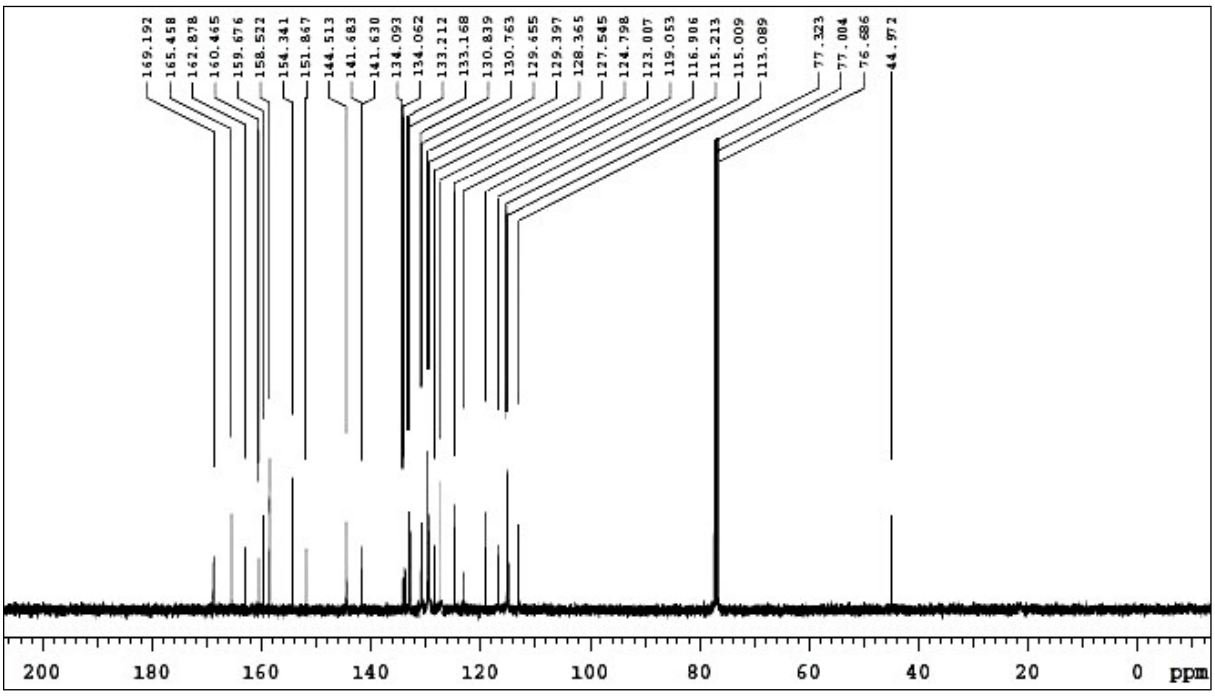
^{13}C NMR spectrum of compound (1i)



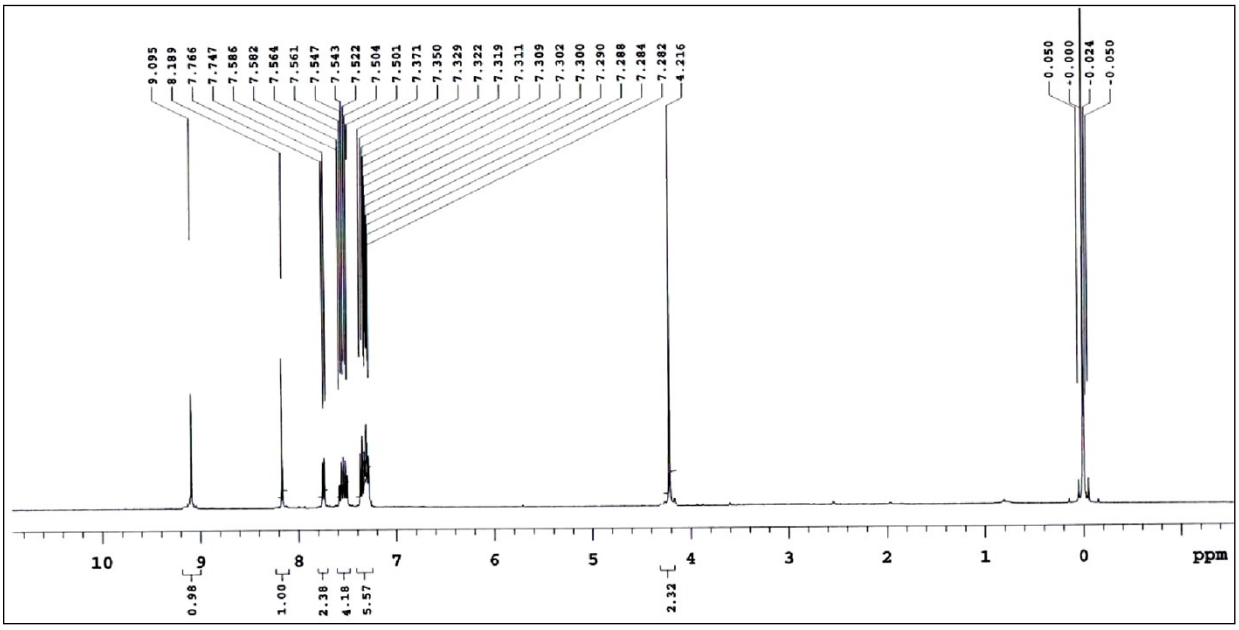
[1]H NMR spectrum of compound (1j)



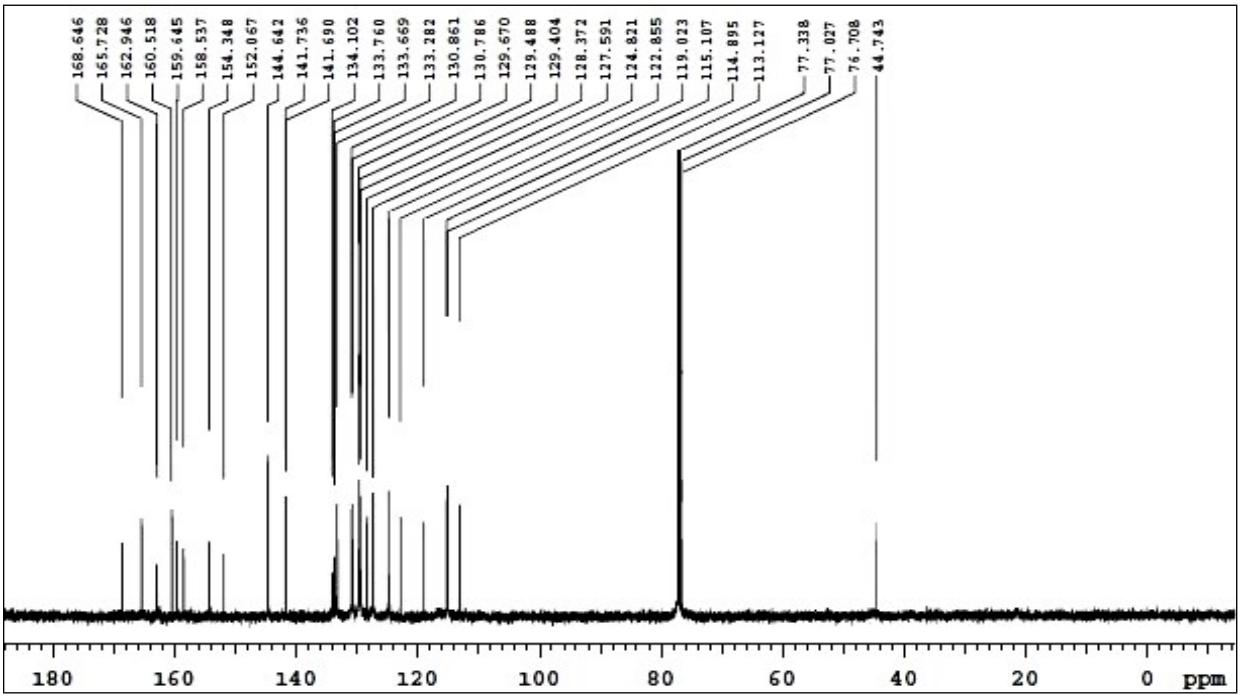
[13]C NMR spectrum of compound (1j)



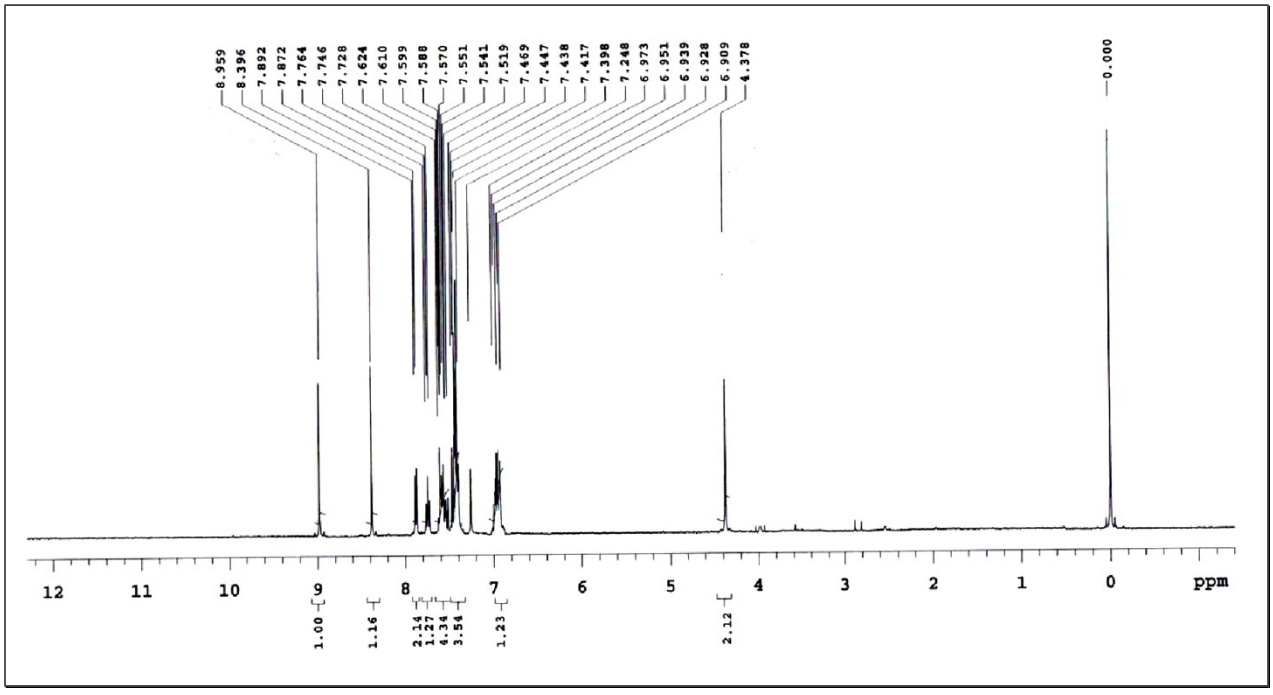
^{1}H NMR spectrum of compound (1k)



^{13}C NMR spectrum of compound (1k)



^{1}H NMR spectrum of compound (1l)



^{13}C NMR spectrum of compound (1l)