

Supporting Information

A facile synthesis and evaluation of new biomolecule-based coumarin-thiazoline hybrids as potent anti-tubercular agents their cytotoxicity, DNA cleavage and X-ray studies

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Table S2: Selected Bond lengths (Å) for **(1a)**

S1—C17	1.7705 (19)	C8—C9	1.448 (3)
S1—C19	1.795 (3)	C8—C16	1.509 (2)
S2—C17	1.749 (2)	C9—C10	1.396 (2)
S2—C16	1.801 (2)	C9—C11	1.407 (3)
O3—C6	1.366 (2)	C10—C14	1.378 (3)
O3—C10	1.383 (2)	C11—C12	1.376 (3)
O4—C6	1.210 (2)	C11—H11	0.93
N5—C17	1.255 (3)	C12—C13	1.401 (3)
N5—C18	1.462 (3)	C12—C15	1.505 (3)
C6—C7	1.439 (3)	C13—C14	1.374 (3)
C7—C8	1.340 (3)	C14—H14	0.93
C7—H7	0.93	C18—C19	1.498 (3)

Table S3: Selected Bond angles (°) for **(1a)**

C17—S1—C19	88.60 (10)	C13—C14—H14	120.6
C17—S2—C16	100.45 (9)	C10—C14—H14	120.6
C6—O3—C10	110.88 (18)	C12—C15—H15B	109.5
N5—C17—S2	125.75 (16)	C12—C11—H11	119
C11—C12—C13	118.16 (17)	C11—C12—C15	121.04 (18)
C14—C13—H13	119.1	C18—C19—H19B	110.5
C13—C14—C10	118.86 (17)	H19A—C19—H19B	108.6
C8—C16—S2	115.89 (13)	S2—C16—H16A	108.3
C9—C11—H11	119	N5—C17—S1	118.99 (16)
S2—C17—S1	115.23 (11)	N5—C18—C19	111.30 (19)
N5—C18—H18A	109.4	C19—C18—H18A	109.4

Table S5: Selected Bond lengths (Å) for **(1b)**

Cl1—C14	1.7427 (19)	C8—H8	0.93
S2—C17	1.7595 (19)	C9—C10	1.456 (3)
S2—C19	1.790 (3)	C9—C16	1.498 (3)
S3—C17	1.750 (2)	C10—C11	1.395 (3)
S3—C16	1.7991 (18)	C10—C15	1.400 (2)
O4—C7	1.363 (3)	C11—C12	1.381 (3)
O4—C11	1.375 (2)	C12—C13	1.370 (3)
O5—C7	1.205 (3)	C12—H12	0.93
N6—C17	1.264 (3)	C13—C14	1.387 (3)
N6—C18	1.449 (3)	C13—H13	0.93
C7—C8	1.445 (3)	C14—C15	1.373 (3)
C8—C9	1.341 (3)	C15—H15	0.93

Table S6: Selected Bond angles (°) for **(1b)**

C17—S2—C19	89.31 (12)	C15—C14—Cl1	119.43 (15)
C17—S3—C16	100.73 (9)	C13—C14—Cl1	118.84 (15)
C7—O4—C11	121.50 (16)	C14—C15—C10	119.60 (17)
C17—N6—C18	111.0 (2)	C14—C15—H15	120.2
O5—C7—O4	117.3 (2)	C10—C15—H15	120.2
O5—C7—C8	125.2 (2)	C9—C16—S3	116.35 (13)
O4—C7—C8	117.54 (17)	C9—C16—H16A	108.2
C9—C8—C7	122.9 (2)	S3—C16—H16A	108.2
C9—C8—H8	118.5	C9—C16—H16B	108.2
C7—C8—H8	118.5	S3—C16—H16B	108.2
N6—C17—S3	125.82 (15)	N6—C17—S2	119.01 (16)
S3—C17—S2	115.13 (12)	N6—C18—C19	112.7 (2)

Table S8: Selected Bond lengths (Å) for **(1e)**

S1-C8	1.7455(18)	S1-C7	1.8140(18)
N1-C9	1.468(2)	C1-C2	1.503(3)
C1-H1A	0.96	C1-H1B	0.96
C2-C13	1.400(2)	C3-C4	1.378(2)
C6-C11	1.340(2)	C6-C7	1.504(2)
C7-H7A	0.97	C7-H7B	0.97
C9-C10	1.521(3)	C9-H9A	0.97
C10-H10B	0.97	C11-C12	1.445(2)
C11-H11	0.93	C13-C14	1.373(2)
C13-H13	0.93	C14-H14	0.93

Table S9: Selected Bond angles (°) for **(1e)**

C8-S1-C7	102.04(8)	C8-S2-C10	88.64(9)
H1A-C1-H1C	109.5	H1B-C1-H1C	109.5
C3-C2-C13	118.31(16)	C3-C2-C1	120.81(16)
C13-C2-C1	120.88(17)	C4-C3-C2	120.36(15)
C4-C3-H3	119.8	C2-C3-H3	119.8
O1-C4-C3	116.44(13)	O1-C4-C5	121.45(14)
C3-C4-C5	122.10(14)	C4-C5-C14	117.08(15)
C4-C5-C6	117.96(14)	C14-C5-C6	124.95(14)
C6-C7-H7B	109.0	S1-C7-H7B	109.0
N1-C9-C10	110.41(16)	N1-C9-H9A	109.6
C9-C10-S2	105.18(15)	C9-C10-H10A	110.7
S2-C10-H10A	110.7	C9-C10-H10B	110.7
S2-C10-H10B	110.7	H10A-C10-H10B	108.8
C13-C14-H14	119.6	C5-C14-H14	119.6

Table S11: Selected Bond lengths (Å) for **(1h)**

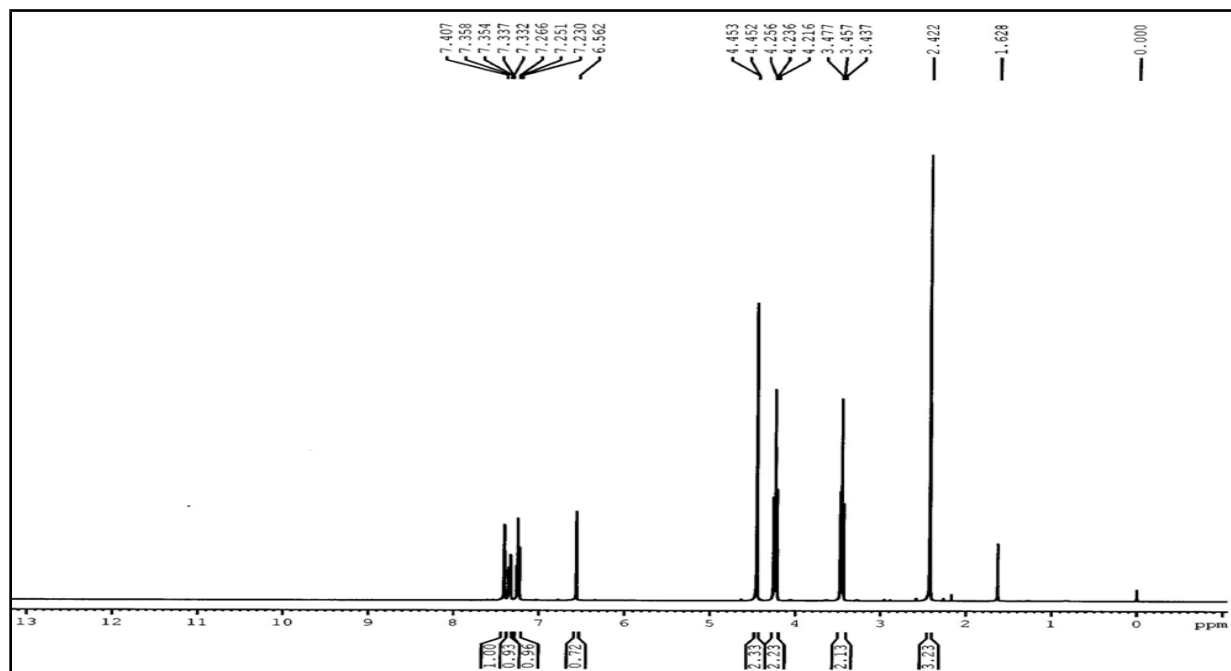
S1-C8	1.752(7)	S1-C7	1.804(7)
O1-C14	1.368(8)	O1-C13	1.375(8)
N1-C9	1.479(8)	C1-C2	1.510(9)
C1-H1A	0.96	C1-H1B	0.96
C2-C3	1.388(10)	C3-C4	1.381(9)
C5-C6	1.459(9)	C6-C15	1.321(9)
C6-C7	1.524(9)	C7-H7A	0.97
C11-H11A	0.96	C11-H11B	0.96
C11-H11C	0.96	C12-C13	1.359(9)
C12-H12	0.93	C14-C15	1.442(9)

Table S12: Selected Bond angles (°) for **(1h)**

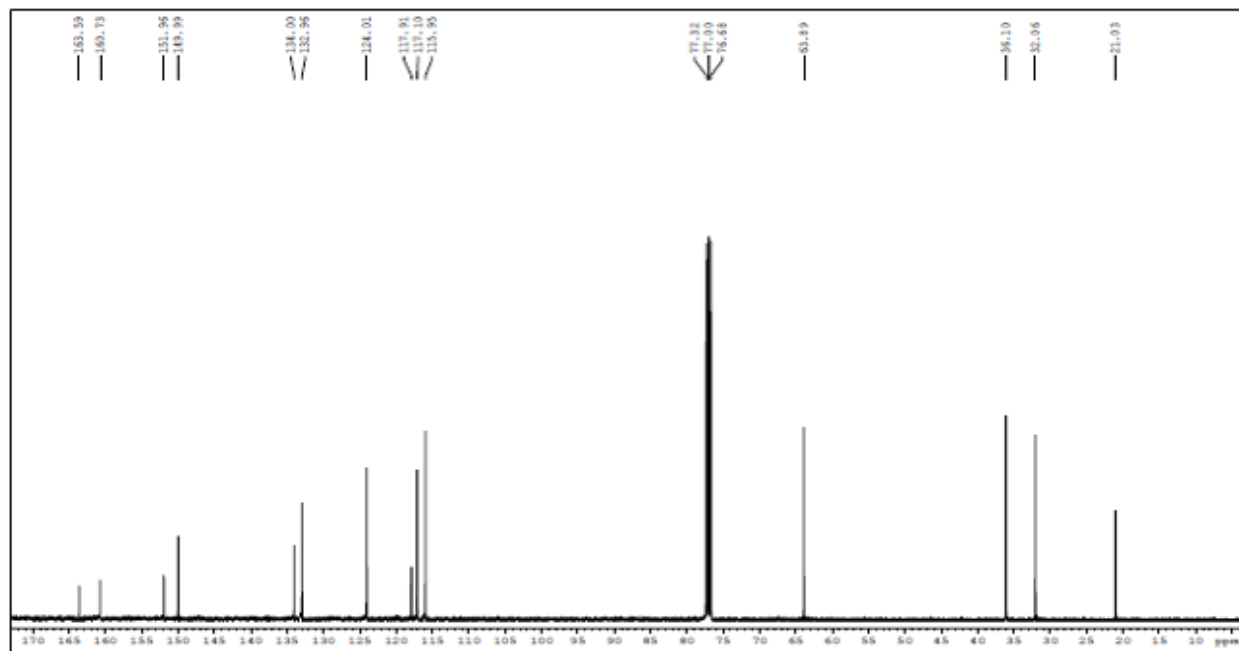
C8-S1-C7	99.0(3)	C8-S2-C10	87.9(4)
C14-O1-C13	122.7(5)	C8-N1-C9	109.5(6)
C2-C1-H1A	109.5	C2-C1-H1B	109.5
C3-C2-C1	120.7(7)	C4-C3-C2	123.4(7)
C4-C3-H3	118.3	C2-C3-H3	118.3
C15-C6-C5	119.4(6)	C15-C6-C7	119.7(6)
C6-C7-H7B	109.1	S1-C7-H7B	109.1
H7A-C7-H7B	107.9	N1-C8-S1	126.1(6)
N1-C9-C10	110.0(6)	N1-C9-H9A	109.7
C10-C9-H9A	109.7	N1-C9-H9B	109.7
S2-C10-H10B	110.9	H10A-C10-H10B	108.9
O2-C14-O1	117.4(6)	O2-C14-C15	127.6(7)
O1-C14-C15	115.0(7)	C6-C15-C14	124.8(7)
C6-C15-H15	117.6	C14-C15-H15	117.6

^1H and ^{13}C NMR spectra's of compounds (1a-1j)

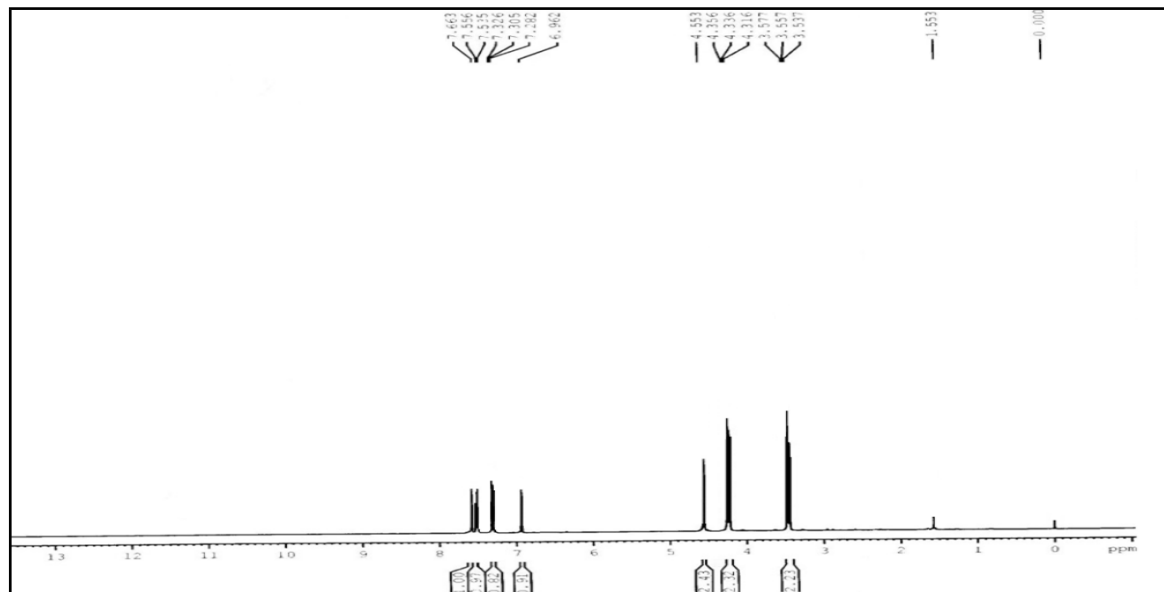
^1H NMR of compound (1a)



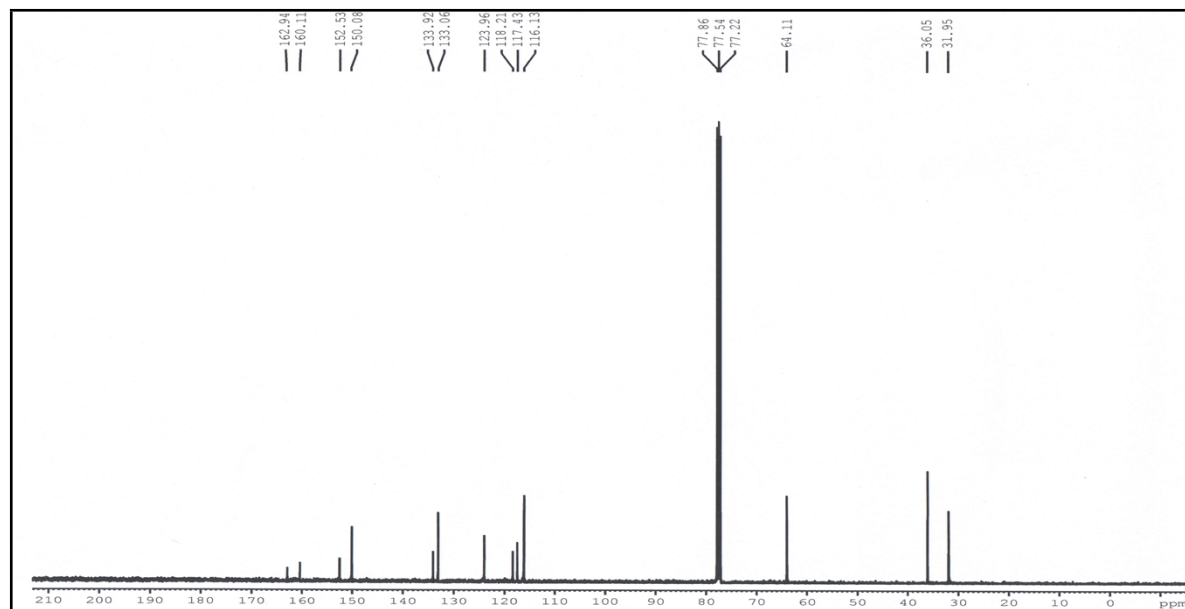
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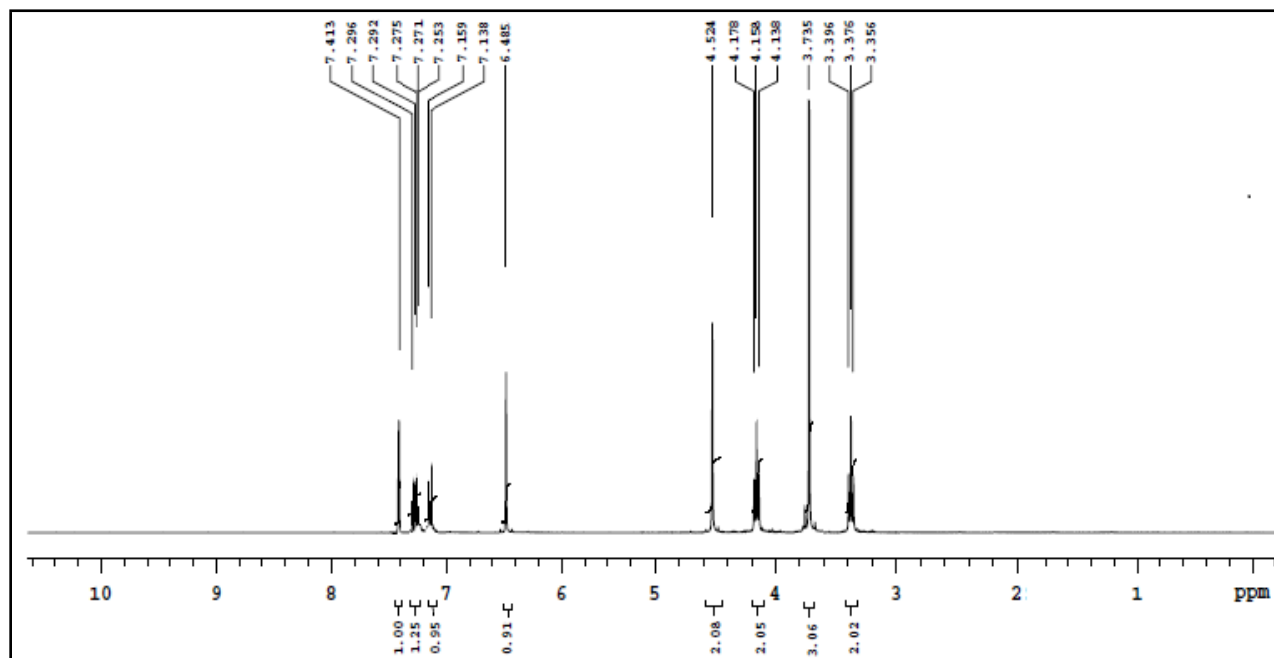
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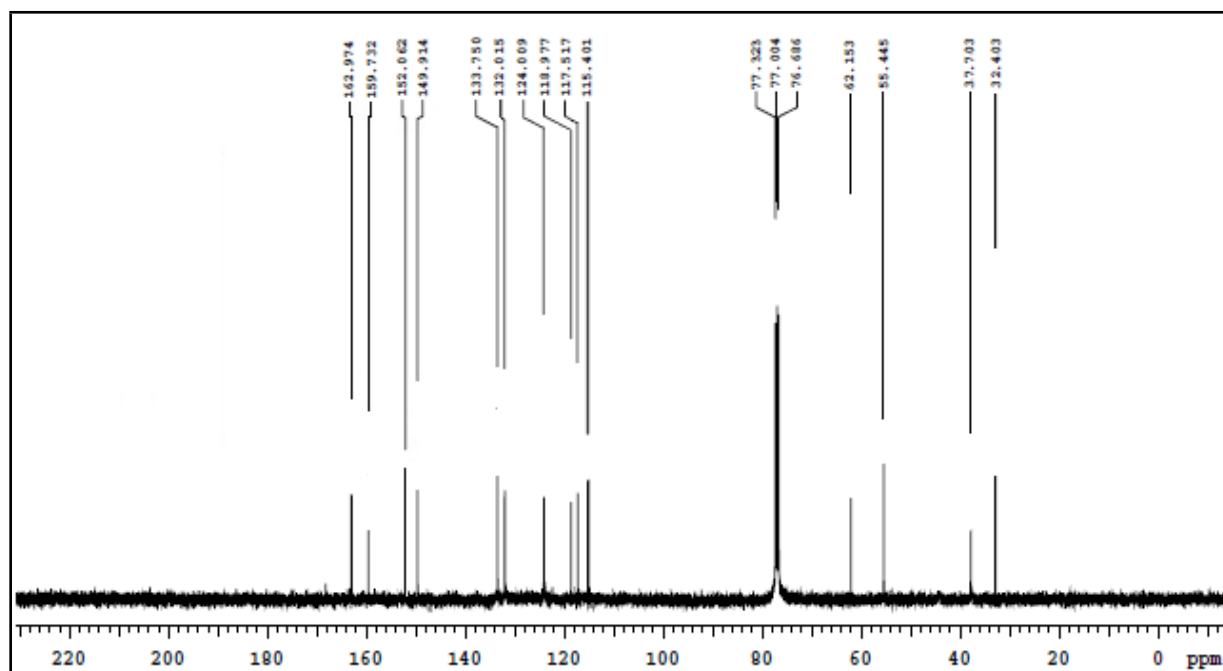
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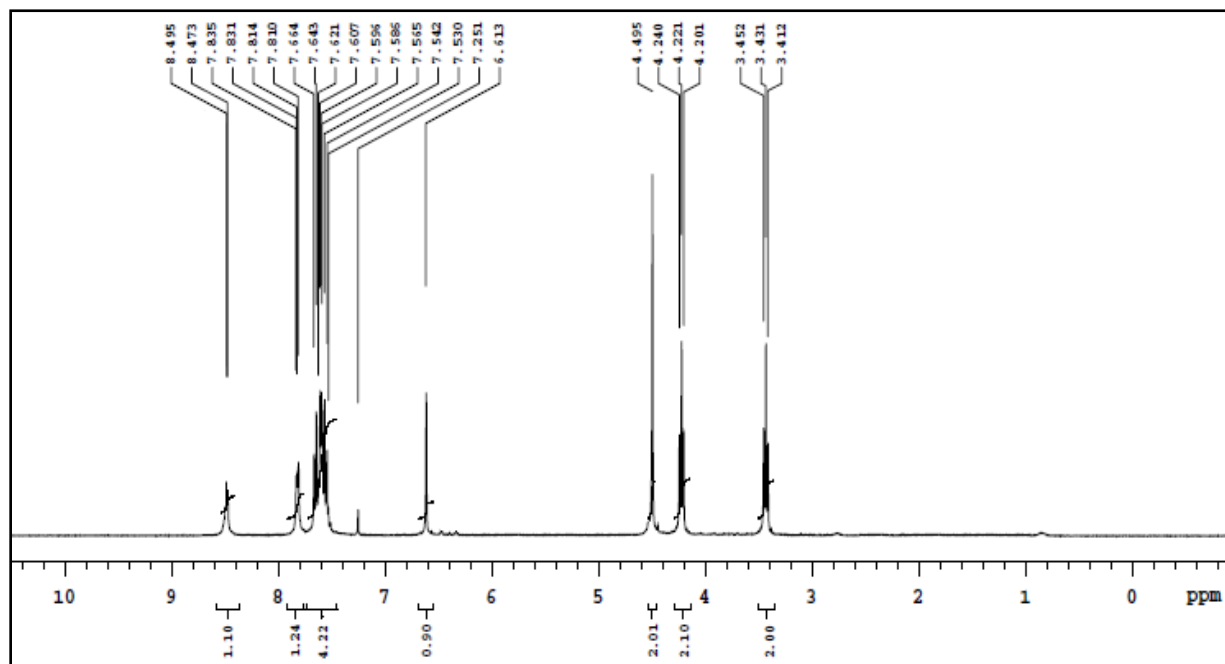
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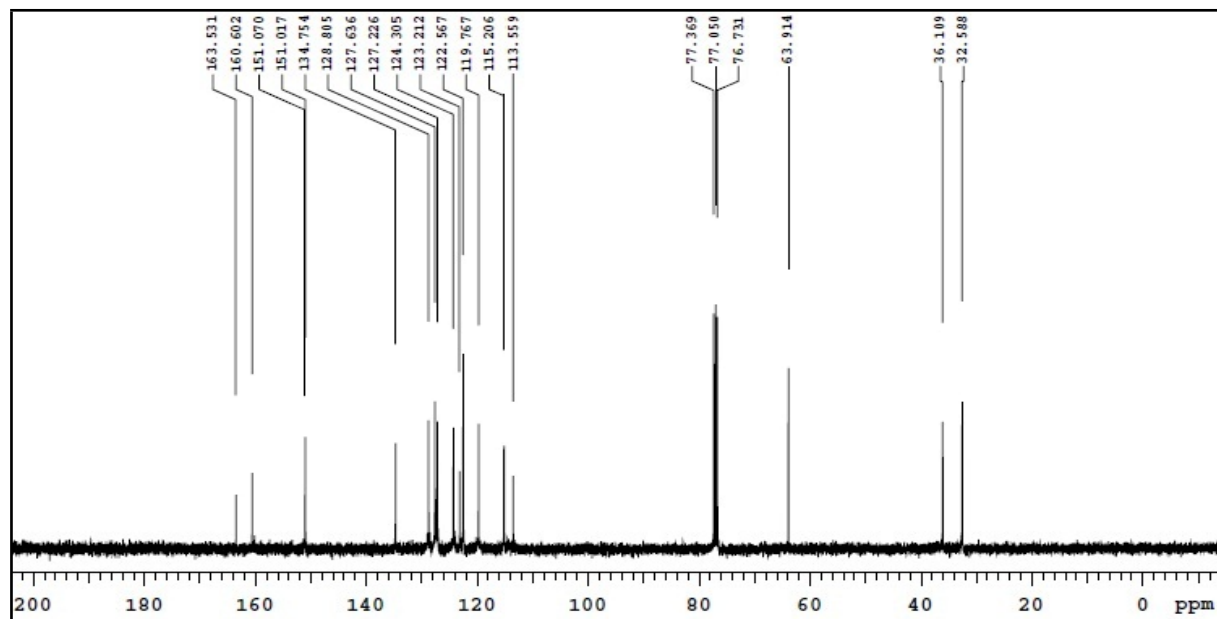
^{13}C NMR of compound (**1c**)



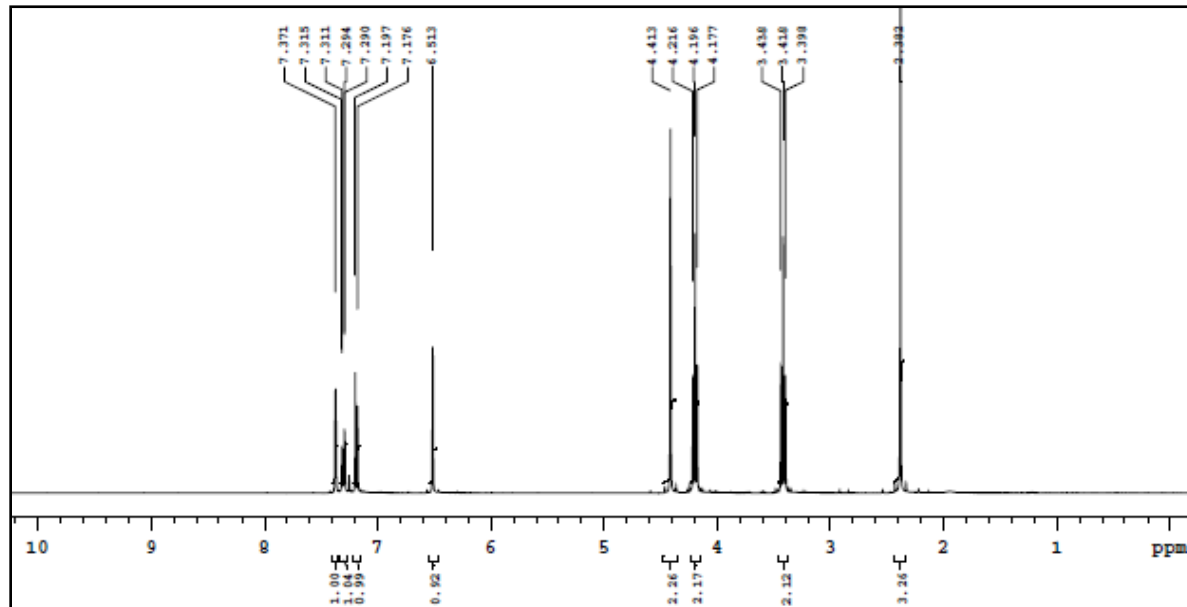
^1H NMR of compound (**1d**)



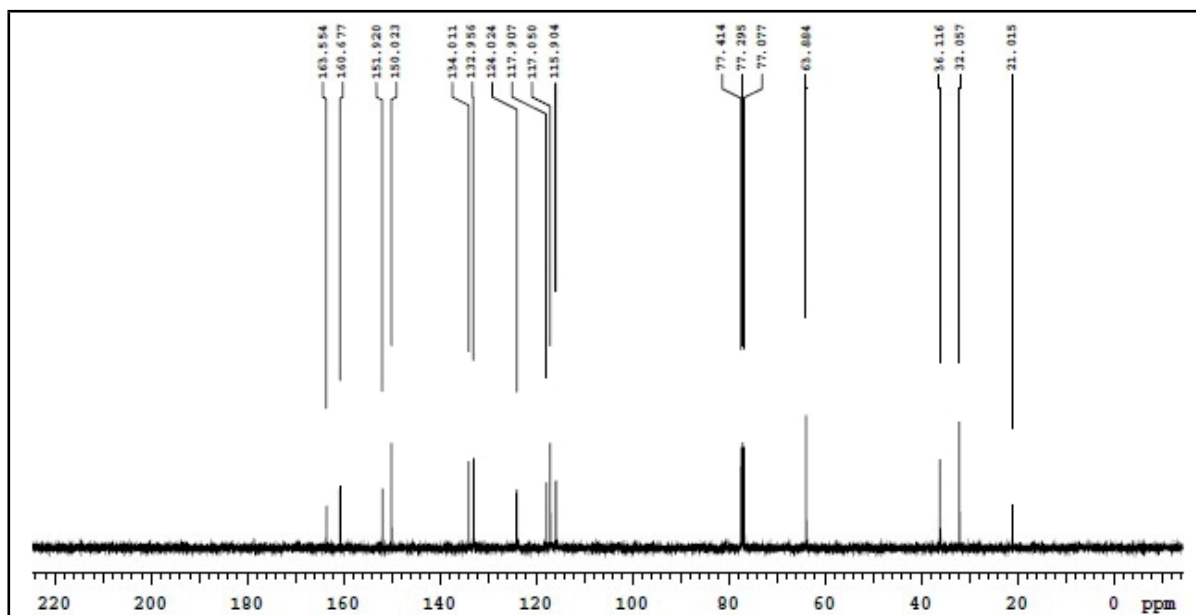
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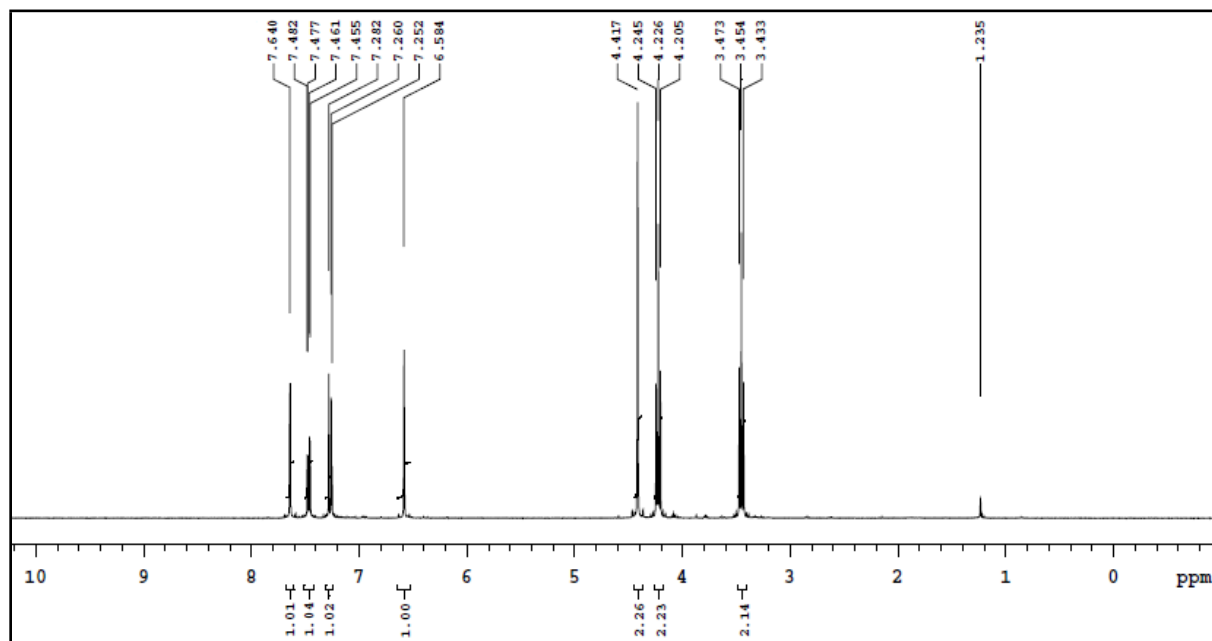
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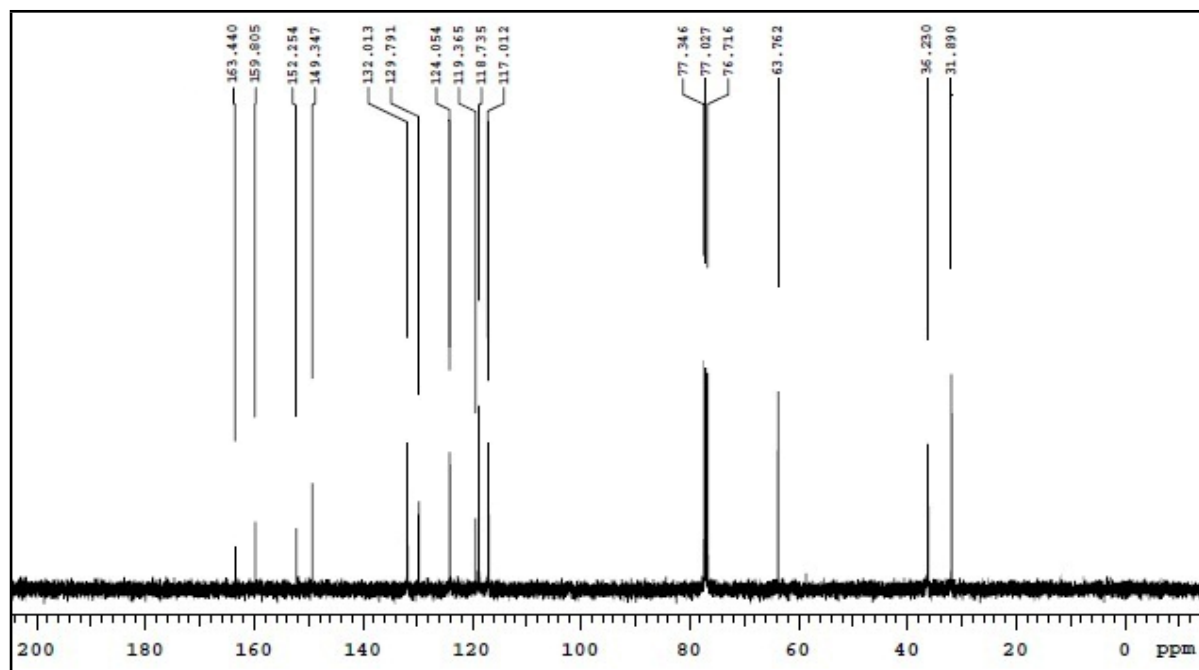
^{13}C NMR of compound (**1e**)



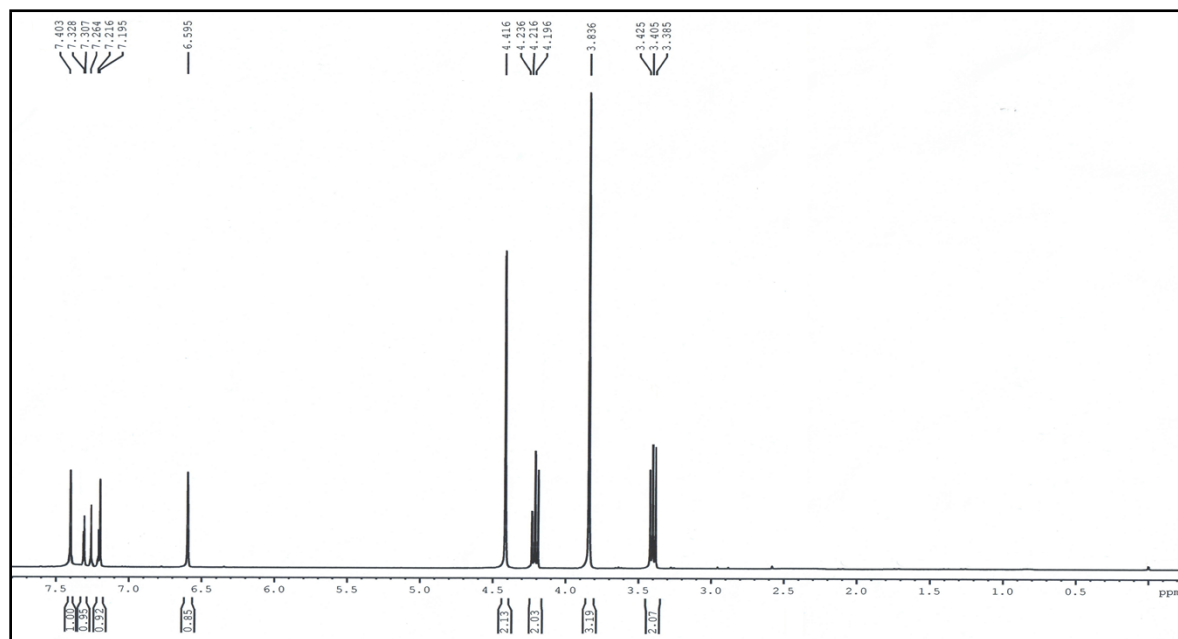
^1H NMR of compound (**1f**)



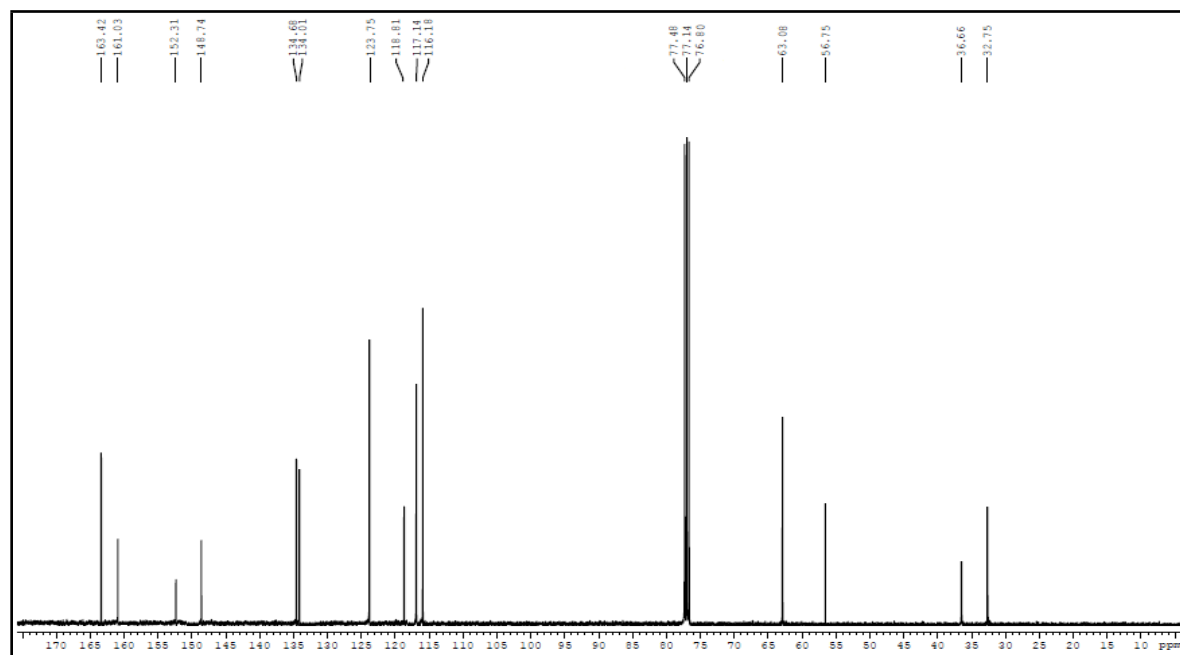
^{13}C NMR of compound (**1f**)



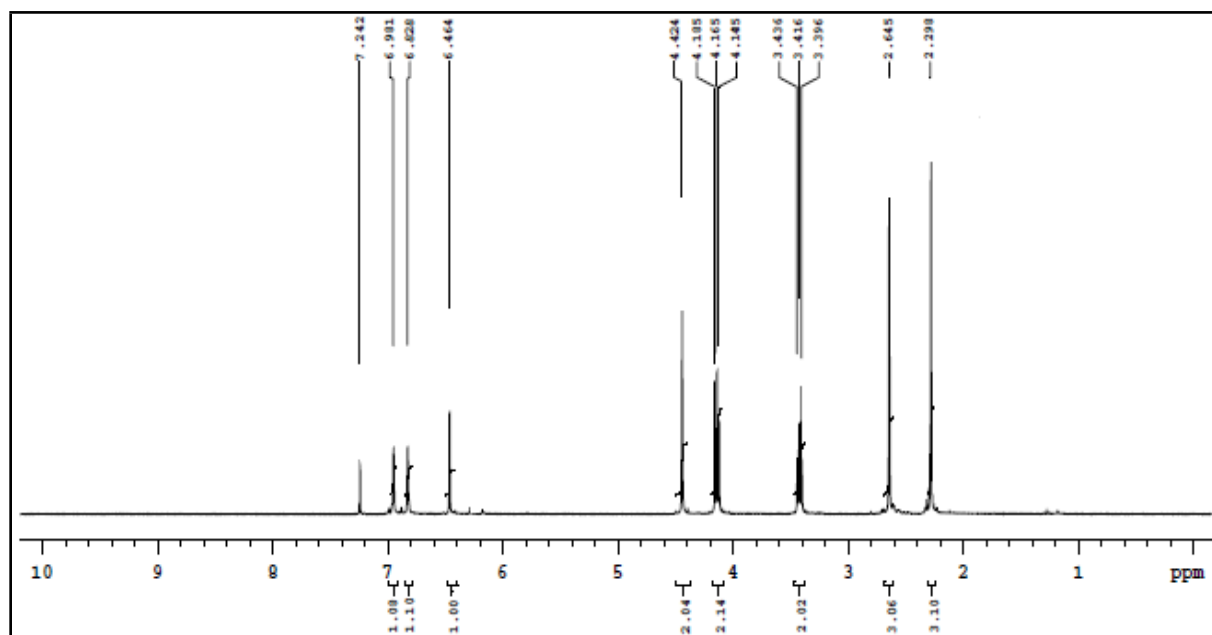
^1H NMR of compound (**1g**)



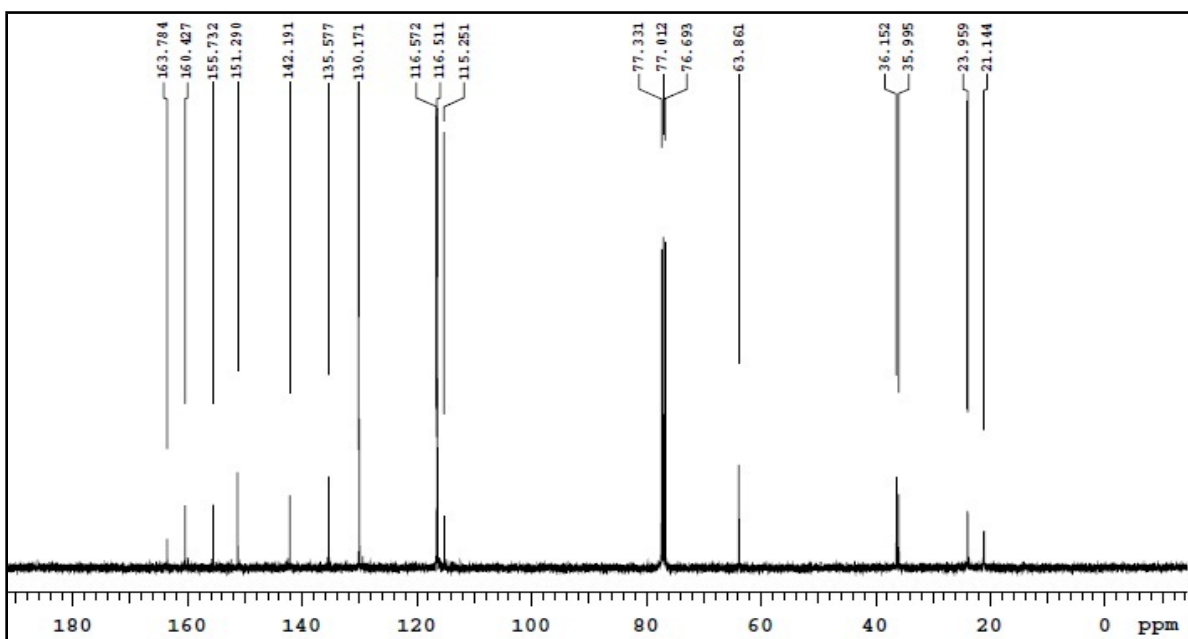
^{13}C NMR of compound (**1g**)



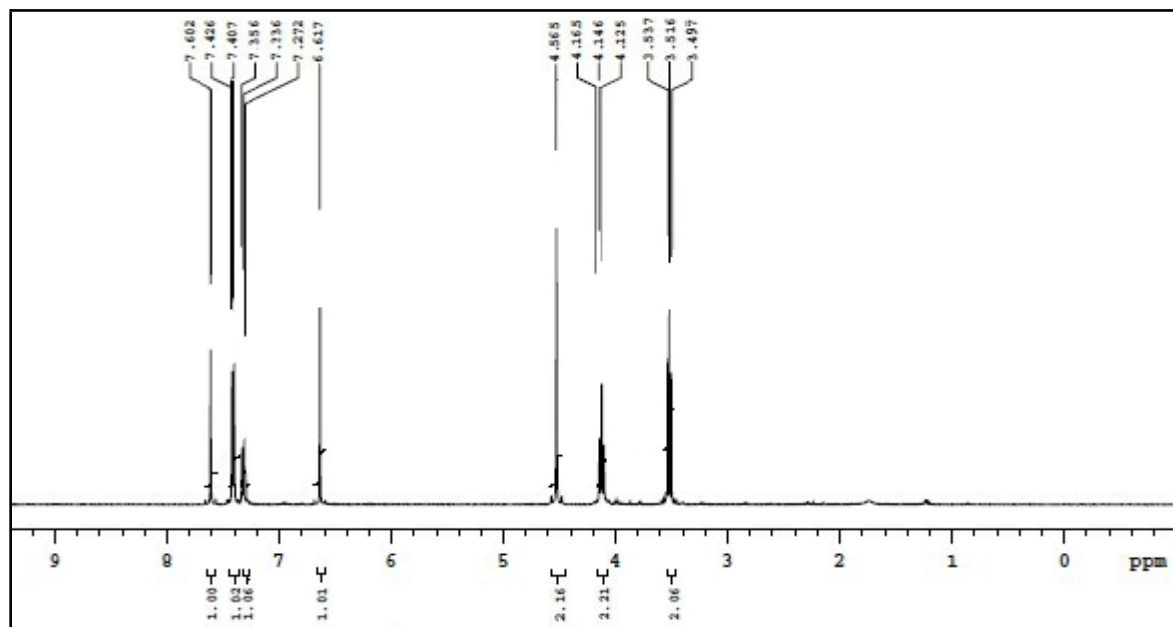
^1H NMR of compound (**1h**)



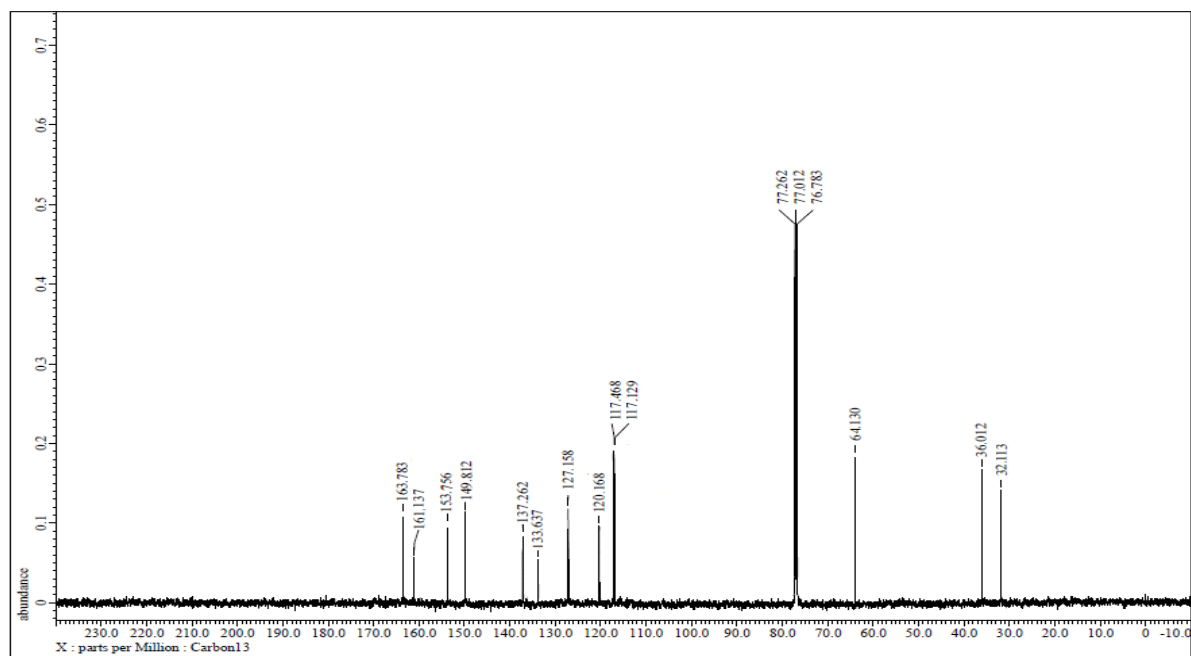
^{13}C NMR of compound (**1h**)



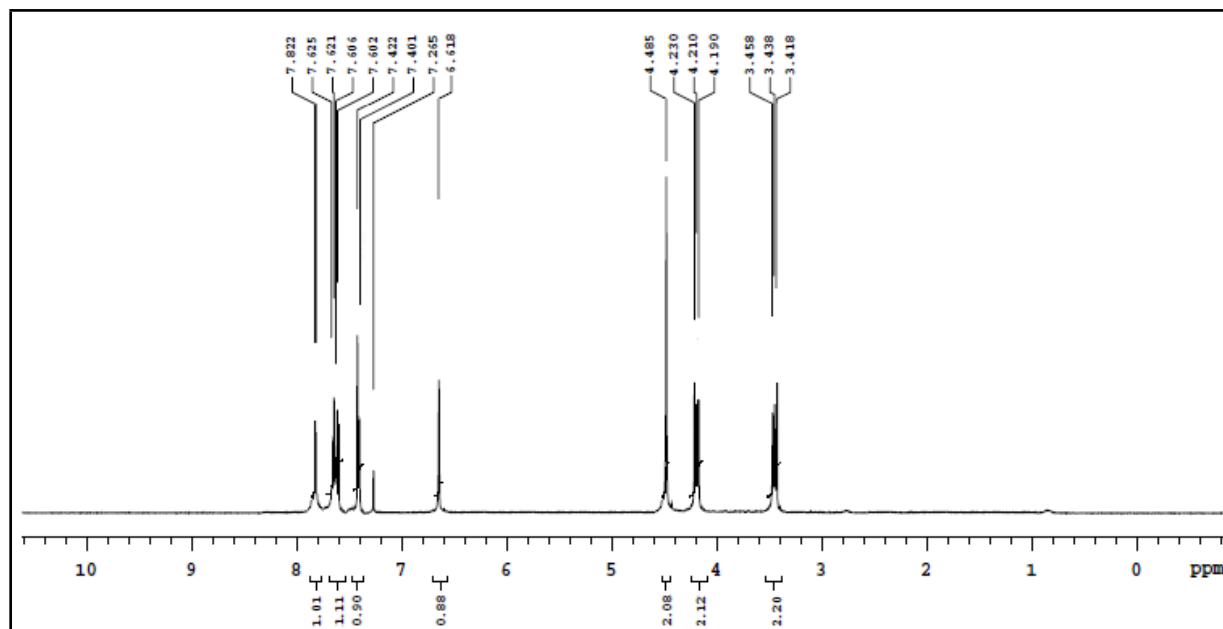
^1H NMR of compound (**1i**)



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



^1H NMR of compound (**1j**)



^{13}C NMR of compound (**1j**)

