

Supplementary Material

Synthesis of 1,2,3-triazole-bound-1,2,4-triazoles containing N-phenylmorpholine structure: antibacterial, antifungal, and antioxidant properties, and AChE-inhibition analysis

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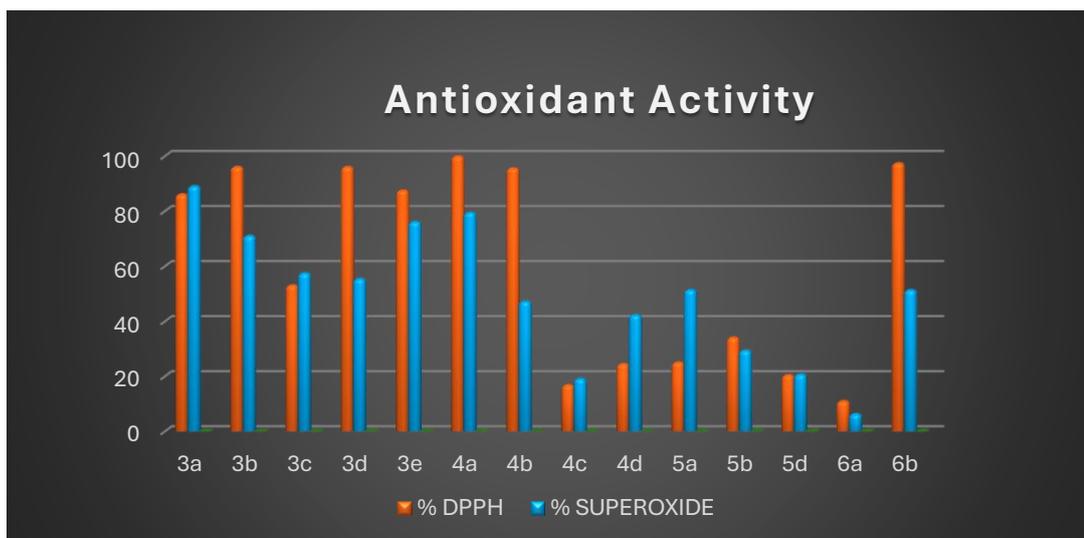
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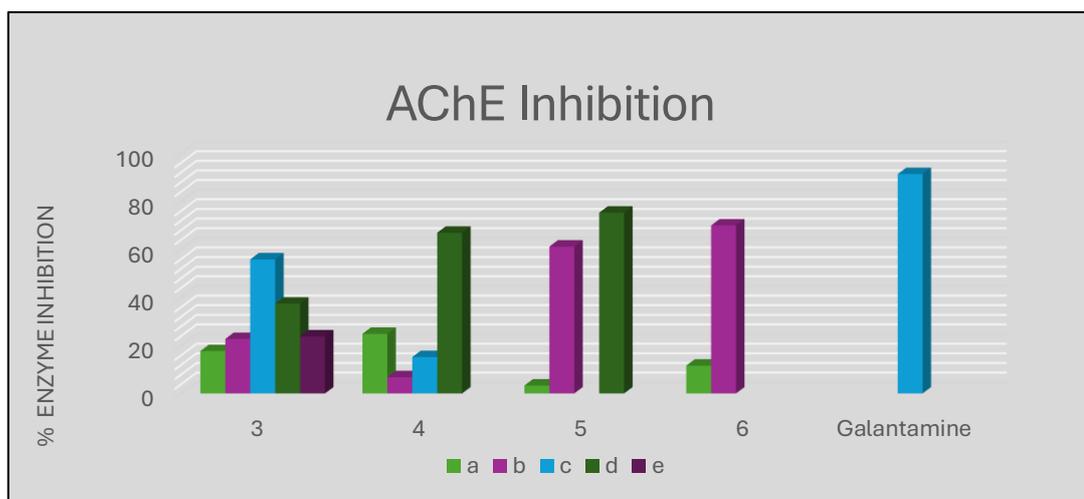
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S1. Results of comparative antioxidant activity



S2. Acetylcholinesterase graphical inhibition results

Table1: Antifungal inhibition zone values of the compounds

Comp.	<i>S. aureus</i>	<i>E. coli</i>	<i>C. perfringens</i>	<i>P. aeruginosa</i>	<i>P. vulgaris</i>	<i>K. pneumoniae</i>
3a	11.166±0.57	1.040±0.52	1.112±0.72	1.390±0.29	1.166±0.57	1.51±0.28
3b	0.700±0.00	1.296±0.005	1.21±0.017	1.000±0.00	1.42±0.24	0.833±0.057
3c	1.400±0.00	0.833±0.057	0.600±0.00	0.833±0.057	1.656±0.011	1.626±0.025
3d	0.600±0.00	1.21±0.017	0.600±0.00	0.600±0.00	1.100±0.00	1.033±0.57
3e	1.626±0.05	1.620±0.51	1.233±0.057	1.950±0.51	1.786±0.005	1.786±0.005
4a	1.100±0.00	1.266±0.57	0.836±0.49	1.86±0.112	1.166±0.57	1.033±0.57
4b	1.600±0.00	1.683±0.011	1.000±0.00	1.00±0.00	1.523±0.005	0.700±0.00
4c	1.629±0.044	2.106±0.11	1.233±0.057	0.700±0.00	1.100±0.00	1.626±0.025
4d	1.856±0.051	1.700±0.00	0.700±0.00	1.21±0.017	1.100±0.00	1.626±0.025
5a	1.406±0.02	1.85±0.112	1.662±0.010	1.853±0.047	1.526±0.005	1.296±0.005
5b	1.400±0.00	1.133±0.057	0.600±0.00	1.823±0.04	1.21±0.017	0.600±0.00
5d	1.853±0.005	0.863±0.055	0.700±0.00	1.400±0.00	1.100±0.00	1.400±0.00
6a	1.21±0.17	1.52±0.010	0.600±0.00	1.296±0.005	0.600±0.00	0.600±0.00
6b	1.21±0.017	1.100±0.00	1.033±0.57	1.033±0.57	1.000±0.00	0.600±0.00
Ampicillin	1.00±00	1.500±0.00	4.316±0.028	2.926±0.046	2.900±0.00	1.326±0.023
Cephazolin	0.600±0.00	1.500±0.00	4.316±0.028	2.433±0.028	0.600±0.00	1.100±0.00
Nystatin	-	-	-	-	-	-
Solvents	-	-	-	-	-	-
Comp.	<i>L. monocytogenes</i>	<i>B. subtilis</i>	<i>Candida albicans</i>	<i>Salmonella enteritidis</i>		
3a	1.110 ±0.00	1.36 ±0.57	1.31±0.23	1.100±0.00		
3b	1.21±0.17	1.300±0.00	1.42±0.24	0.700±0.00		
3c	0.700±0.00	0.700±0.00	0.600±0.00	0.900±0.00		
3d	1.266±0.057	1.786±0.005	0.600±0.00	0.900±0.00		
3e	1.400±0.00	1.953±0.046	0.600±0.00	0.600±0.00		
4a	0.900±0.00	1.42±0.24	0.600±0.00	0.700±0.00		
4b	1.033±0.57	1.638±0.034	1.300±00	0.900±0.00		
4c	0.700±0.00	1.550±0.010	1.856±0.051	0.600±0.00		
4d	0.833±0.057	1.926±0.046	2.00±0.00	0.900±0.00		
5a	1.100±0.00	1.823±0.04	1.786±0.005	1.42±0.24		
5b	1.033±0.57	1.950±0.051	1.266±0.057	0.900±0.00		
5d	1.033±0.57	2.060±0.010	2.320±0.026	1.266±0.057		
6a	1.100±0.00	1.730±0.51	1.100±0.00	0.65±0.05		
6b	1.033±0.57	1.616±0.028	1.21±0.017	1.033±0.57		
Ampicillin	2.400±0.00	3.56±0.00	-	3.540±0.034		
Cephazolin	3.313±0.023	3.826±0.109	-	3.516±0.040		
Nystatin	-	-	1.500±0.00	-		
Solvents	-	-	-	-		
Comp.	<i>Streptococcus mutans</i>	<i>Micrococcus luteus</i>	<i>A. niger</i>			
3a	1.120 ±0.72	1.100±0.00	1.11 ±0.10			
3b	0.926±0.046	0.853±0.50	1.100±0.00			
3c	0.700±0.00	0.600±0.00	1.00±0.00			

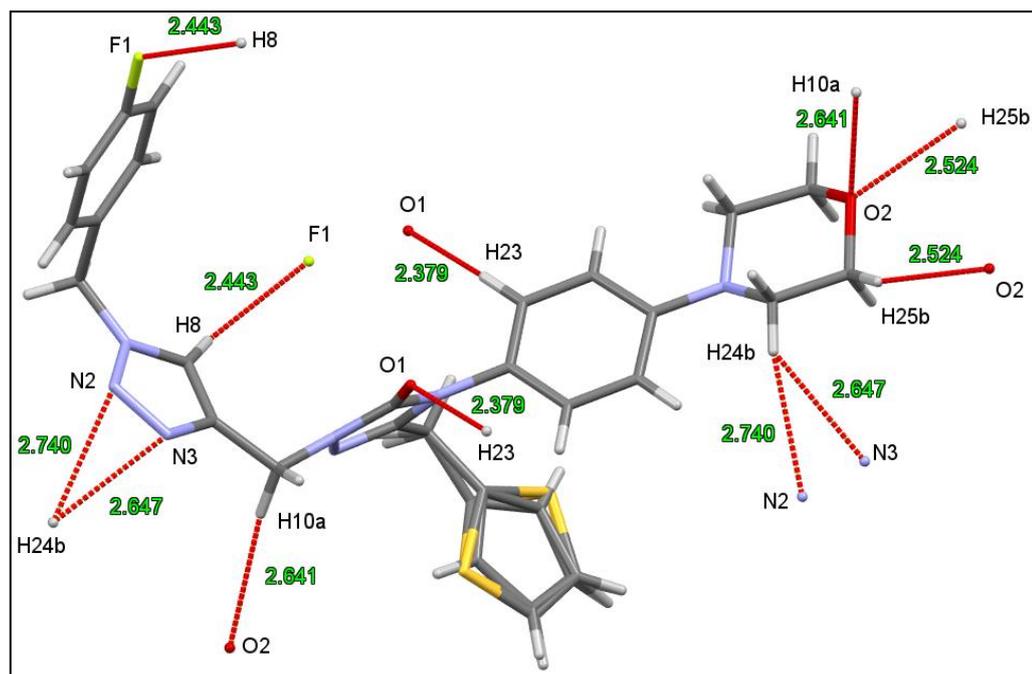
3d	0.600±0.00	0.700±0.00	1.140±0.052
3e	1.306±0.011	0.700±0.00	1.600±0.00
4a	1.21±0.17	0.79±0.05	0.763±0.015
4b	0.900±0.00	0.900±0.00	1.300±0.00
4c	0.900±0.0	2.00±0.00	1.406±0.011
4d	0.600±0.00	2.320±0.026	1.276±0.040
5a	1.42±0.24	0.700±0.00	1.180±0.062
5b	1.400±0.00	0.700±0.00	1.133±0.057
5d	0.600±0.00	1.950±0.051	1.200±0.00
6a	1.033±0.57	0.700±0.00	1.106±0.011
6b	0.900±0.00	0.700±0.00	1.21±0.017
Ampicillin	2.406±0.020	0.600±0.00	-
Cephazolin	3.033±0.057	3.573±0.023	-
Nystatin	-	-	1.600±0.00
Solvents	-	-	-

S3. Table1: Antifungal inhibition zone values of the compounds

Table 2: Experimental (XRD) and optimized geometrical parameters (DFT) of compound (7b)			
Structural parameters			
Bond distance (Å)		XRD	DFT
F1	C1	1.374(5)	1.349
N4	N5	1.389(4)	1.380
N1	N2	1.345(4)	1.354
N1	C8	1.330(4)	1.379
N1	C7	1.465(4)	1.460
N3	N2	1.323(4)	1.305
N3	C9	1.350(4)	1.364
C4	C7	1.510(5)	1.516
C8	C9	1.359(4)	1.379
N5	C12	1.299(4)	1.302
N4	C11	1.360(4)	1.379
O2	C25	1.418(4)	1.424
O1	C11	1.218(4)	1.219
N7	C26	1.457(4)	1.458
N7	C21	1.412(4)	1.384
N6	C12	1.383(4)	1.383
C14A	C15A	1.400(3)	1.368
S1A	C14A	1.680(2)	1.749
S1A	C17A	1.668(19)	1.736
S1B	C17B	1.658(14)	1.736
S1B	C14B	1.694(16)	1.749
Bond angles (°)			
C2	C1	F1	118.6(5)
			118.93

C10	N4	N5		120.9(3)	119.68
C7	N1	C8		129.8(4)	129.48
C12	N5	N4		104.2(3)	104.99
C9	N3	N2		109(3)	109.23
C22	C21	N7		121.8(3)	121.15
N3	N2	N1		106.5(3)	107.37
N5	C12	N6		112.1(3)	111.83
C13	C12	N5		124.7(3)	122.78
N6	C11	O1		127.4(3)	123.67
N4	C11	N6		103.5(3)	102.2
C9	C8	N1		105.8(3)	104.25
C24	C25	O2		111.3(3)	124.29
C9	C10	N4		114.8(3)	113.74
C25	C24	N7		112.9(3)	109.79
C26	C27	O2		111.8(3)	113.3
C24	N7	C21		116.1(3)	116.34
C11	N6	C12		107.3(3)	107.76
C18	N6	C11		126.3(3)	123.67
C16B	C17B	S1B		115.2(10)	111.54
C15B	C14B	S1B		107.9(11)	110.52
C17B	C16B	C15B		108.1(11)	112.69
C17A	S1A	C14A		93.2(12)	91.71
Dihedral bond angle (°)					
N4	C10	C9	C8	20.2(4)	-44.51
N1	N2	N3	C9	0.5(3)	-0.63
N1	C7	C4	C5	-78.7(3)	-54.23
C4	C3	C2	C1	0.4(4)	0.26
F1	C1	C6	C5	178.1(3)	179.8
O2	C27	C26	N7	-55.5(3)	-58.92
O1	C11	N4	N5	179.6(3)	179.78
N4	N5	C12	C13	173.9(2)	176.7
N7	C21	C20	C19	-179.4(3)	-179
N6	C11	N4	C10	169.4(2)	179.77
N5	C12	C13	C14A	-88.2(11)	-106.96
C12	C13	C14A	C15A	-133.3(19)	-117.21
C13	C14A	S1A	C17A	-170(2)	-179.28
N6	C12	C13	C14B	71.4(7)	69.63

S4. Table 2: Experimental (XRD) and optimized geometrical parameters (DFT) of compound (7b)



S5. The crystal packing of the studied compound intermolecular hydrogen bonds

Table 3: Hydrogen bond distances and angles

D—H...A	D—H (Å)	H...A (Å)	D...A (Å)	D—H...A (°)
C23—H23...O1 ^{#1}	0.930	2.379	3.253	156.54
C8—H8...F1 ^{#2}	0.930	2.443	3.213	140.12
C24—H24B...N2 ^{#3}	0.970	2.740	2.786	82.55
C24—H24B...N3 ^{#4}	0.970	2.647	3.431	138.16
C10—H10A...O2 ^{#5}	0.970	2.641	3.595	168.28
C25—H25B...O2 ^{#6}	0.970	2.524	3.424	154.46

D: Donor; A: Acceptor

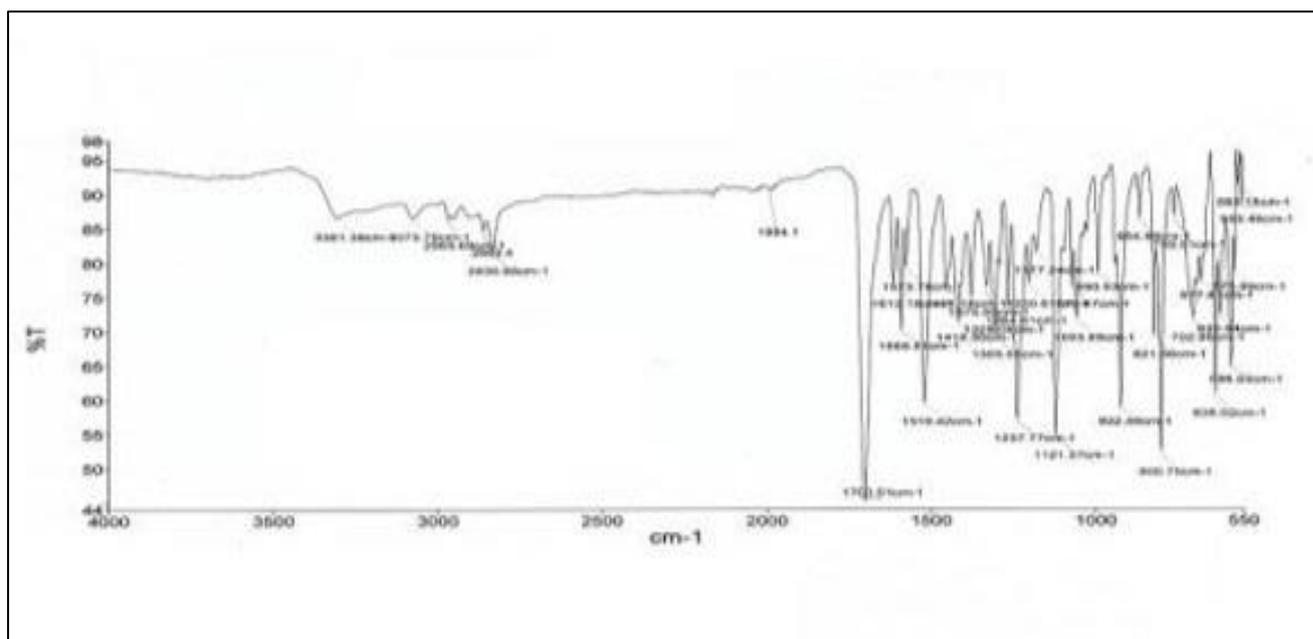
Symmetry codes: $x-1, y, z$ ^{#1}; $x-1/2, -y+1/2+1, -z+1$ ^{#2}; x, y, z ^{#3}; $-x+1/2+1, -y+1, z-1/2$ ^{#4}; $-x+1, y-1/2, -z+1/2$ ^{#5}; $x+1/2, -y+1/2+1, -z$ ^{#6}

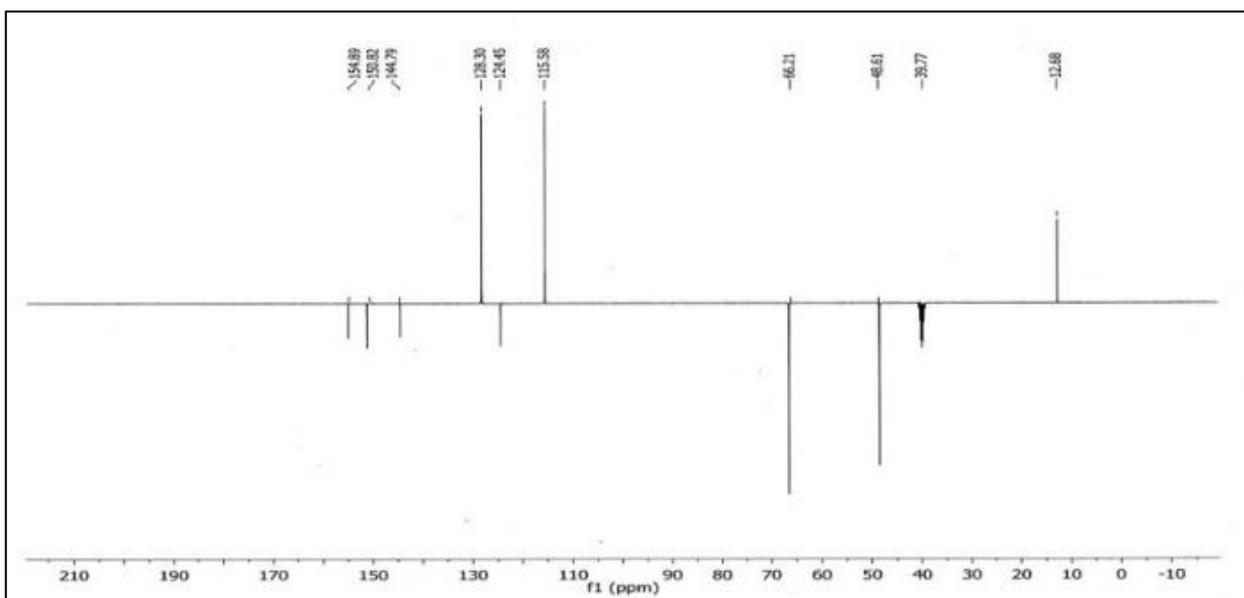
S6. Table 3: Hydrogen bond distances and angles

Table 4: Crystallographic parameters for the C₂₇H₂₆FN₇O₂S (7b) single crystal

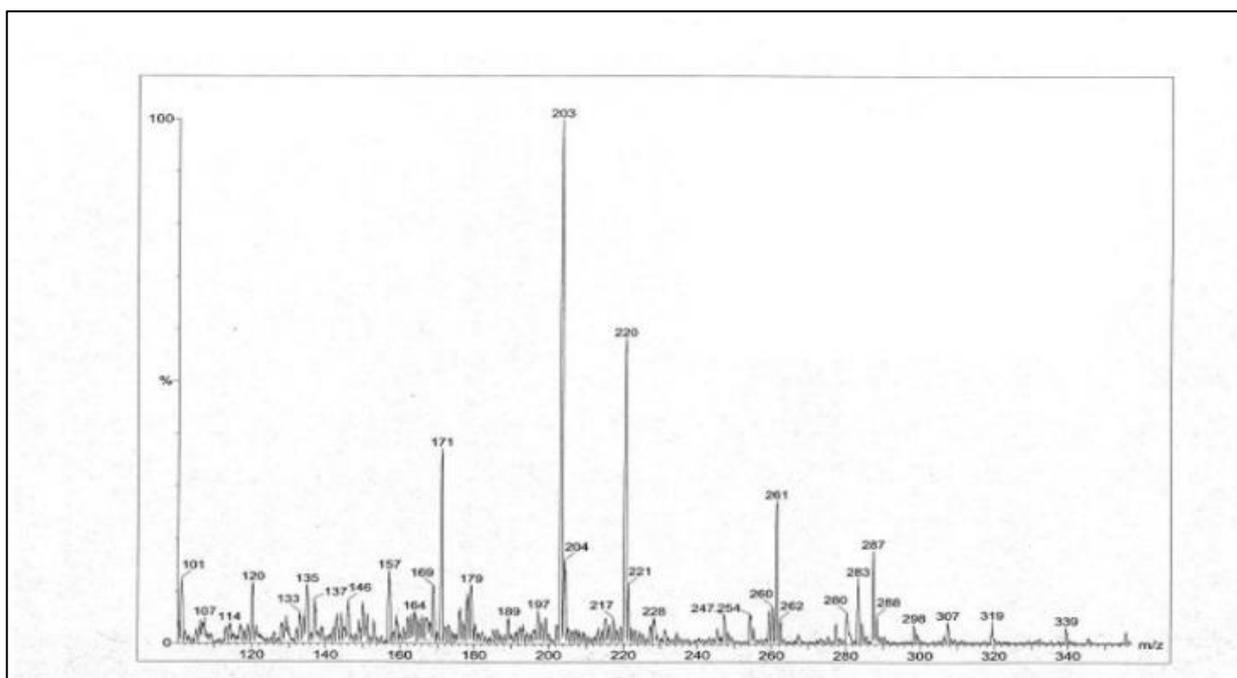
CCDC deposition number	2403655
Chemical formula	C ₂₇ H ₂₆ FN ₇ O ₂ S
Formula weight	531.618
Wavelength	Mo K _α radiation, λ=0.71073 Å
Temperature	293.15 K
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
Crystal color	colourless
a, b, c	5.8401 (7), 17.074 (2), 25.685 (3) (Å)
α, β, γ	90, 90, 90 (°)
Volume	2561.2 (5) Å ³
Z	4
Density	1.379 g/cm ³
μ	0.174 mm ⁻¹
Absorption correction.	Multi-scan
F ₀₀₀	1113.2
Diffractometer/ meas. meth.	Bruker APEX-II CCD / φ and ω scans
Crystal size	0.1 × 0.05 × 0.04 mm ³
2θ range for data collection	3.18 to 50.98 (°)
Index ranges	-7 ≤ h ≤ 6, -21 ≤ k ≤ 21, -32 ≤ l ≤ 32
T _{min} , T _{max}	0.652, 0.745
Reflections collected	33102
Independent/observed reflections	4729, 2465
R _{int} / R _{sigma}	0.0930 / 0.1362
Final R indexes [I >=2σ(I)]	R ₁ =0.0500, wR ₂ =0.0795
R indices (all data)	R ₁ =0.1511, wR ₂ =0.1065
Data/restraints/parameters	4729 / 45 / 368
Goodness-of-fit on F ²	1.013
Δρ _{max} , Δρ _{min}	0.45, -0.51 (e/Å ³)

S7. Table 4: Crystallographic parameters for the C₂₇H₂₆FN₇O₂S (7b) single crystal

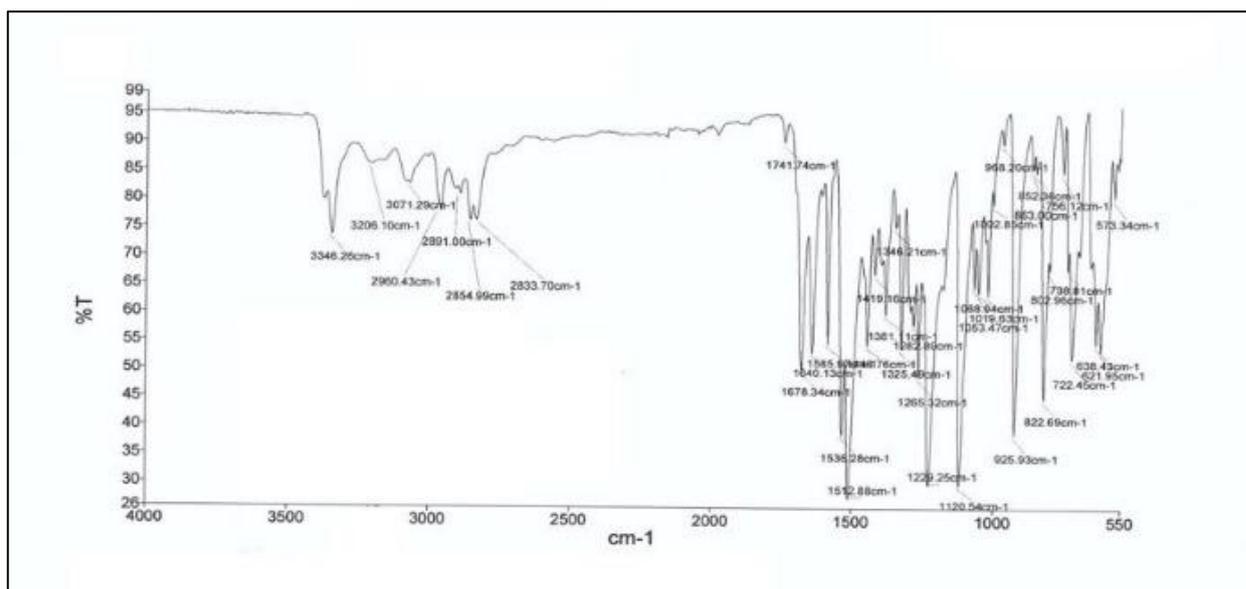
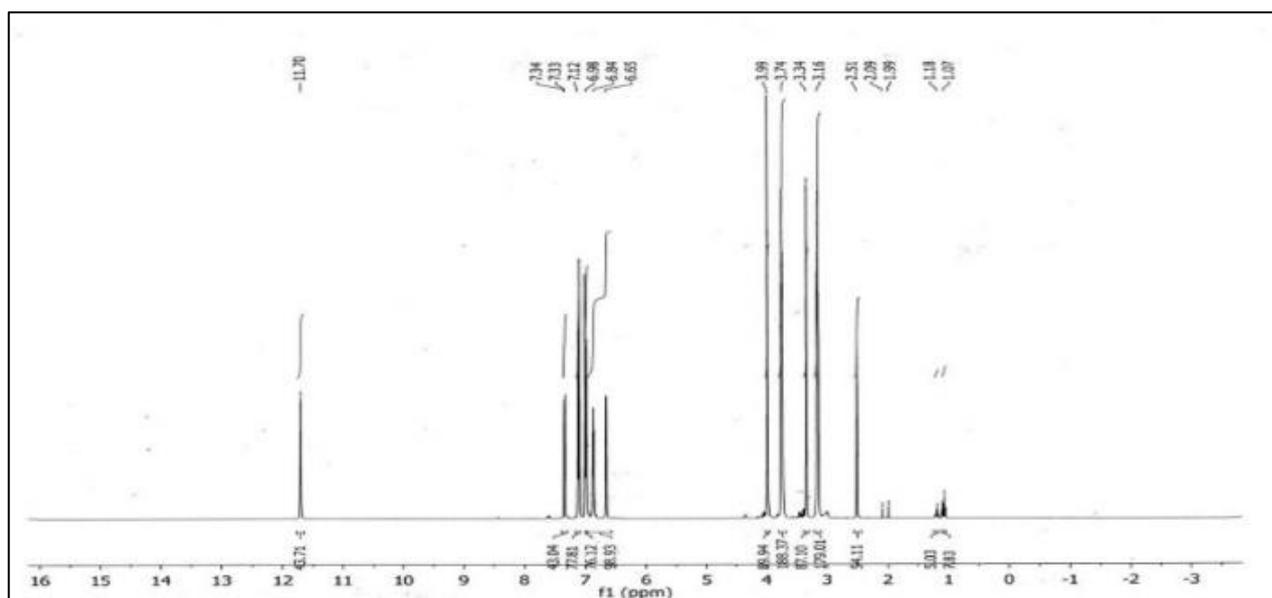


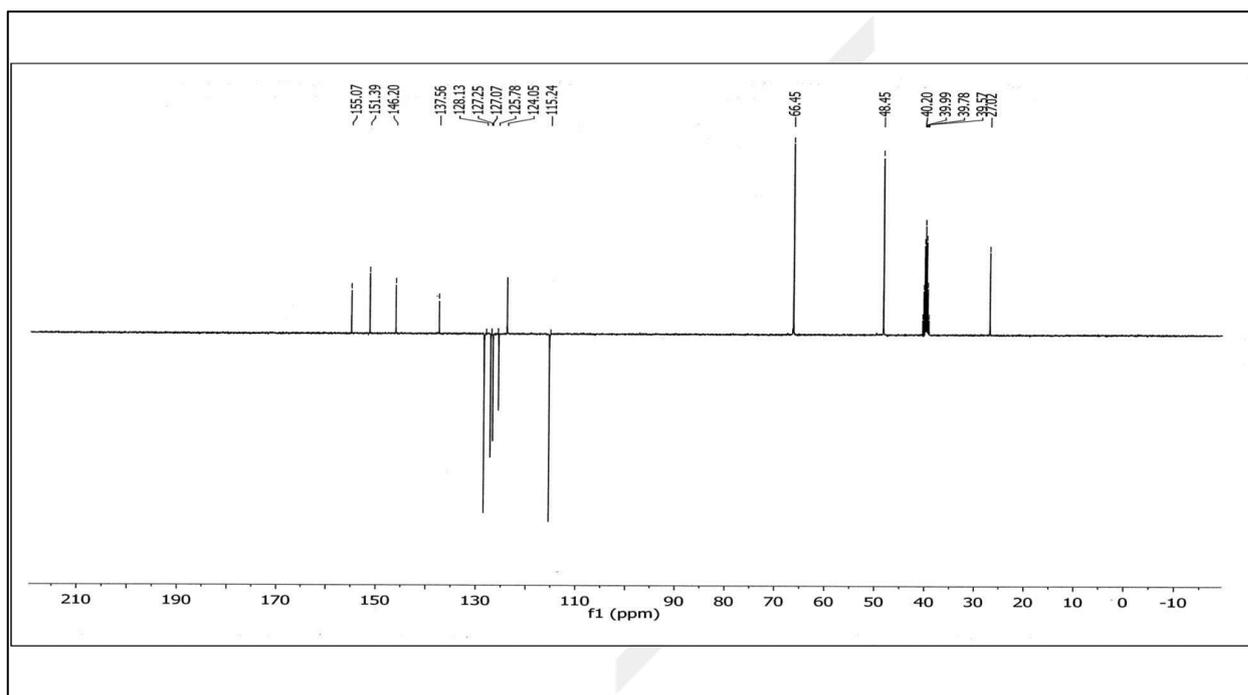


S10. ^{13}C NMR (APT) spectra of compound (3a)

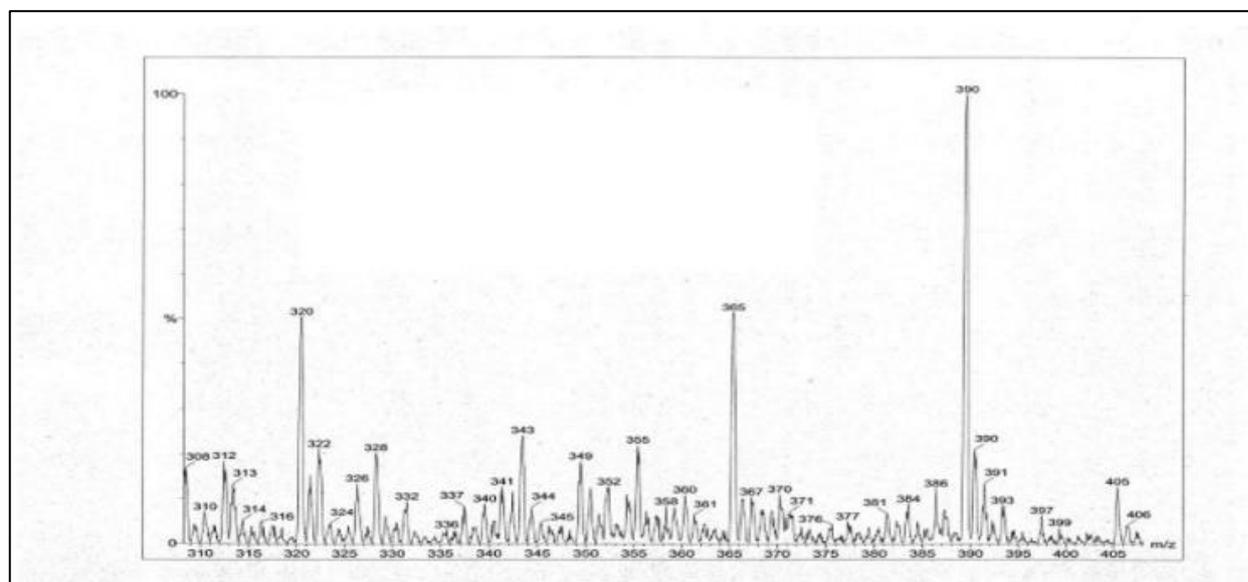


S11. Mass spectra of compound (3a)

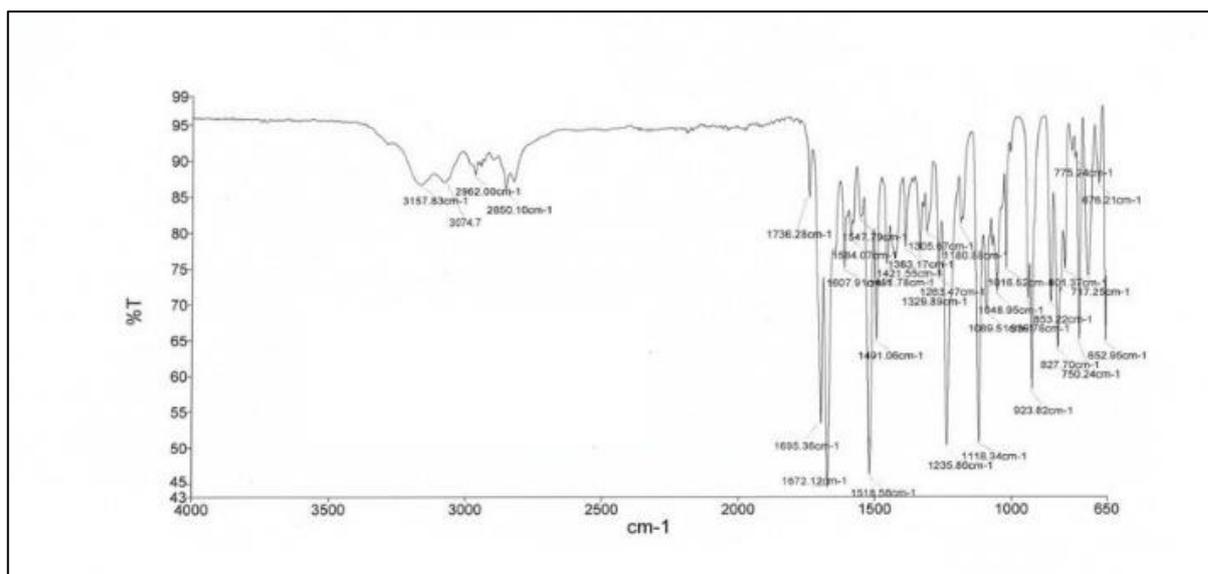
**S12.** FT-IR spectra of compound (3b)**S13.** ¹H NMR spectra of compound (3b)



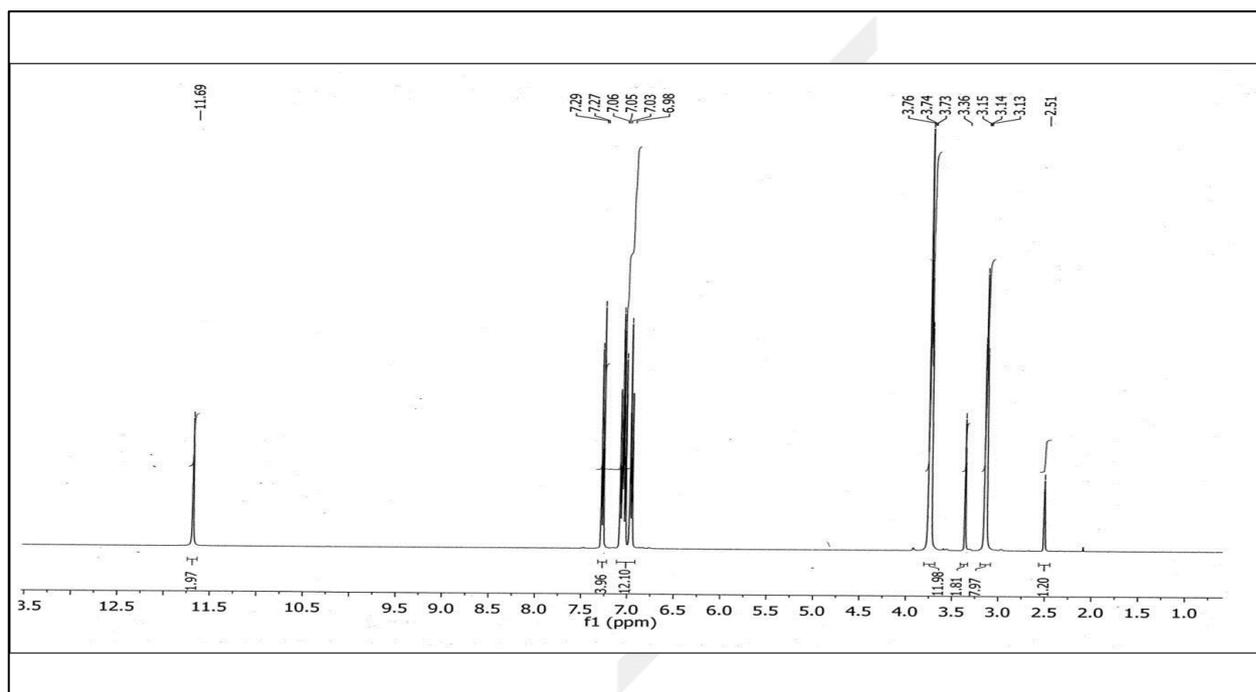
S14. ^{13}C NMR (APT) spectra of compound (3b)

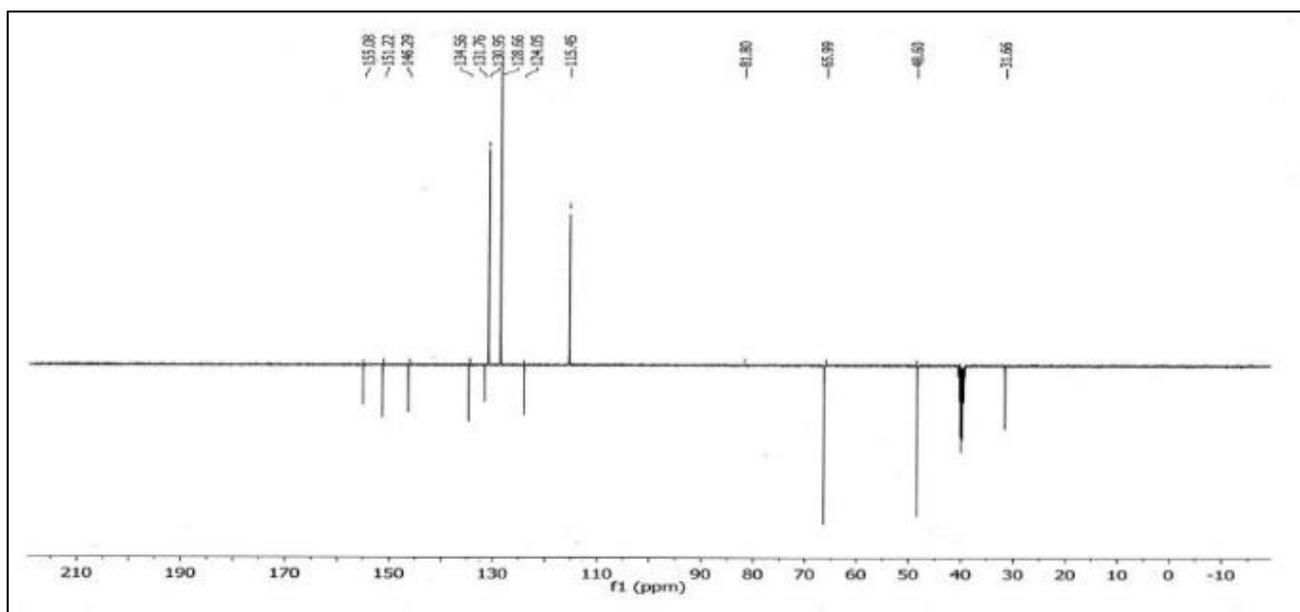


S15. Mass spectra of compound (3b)

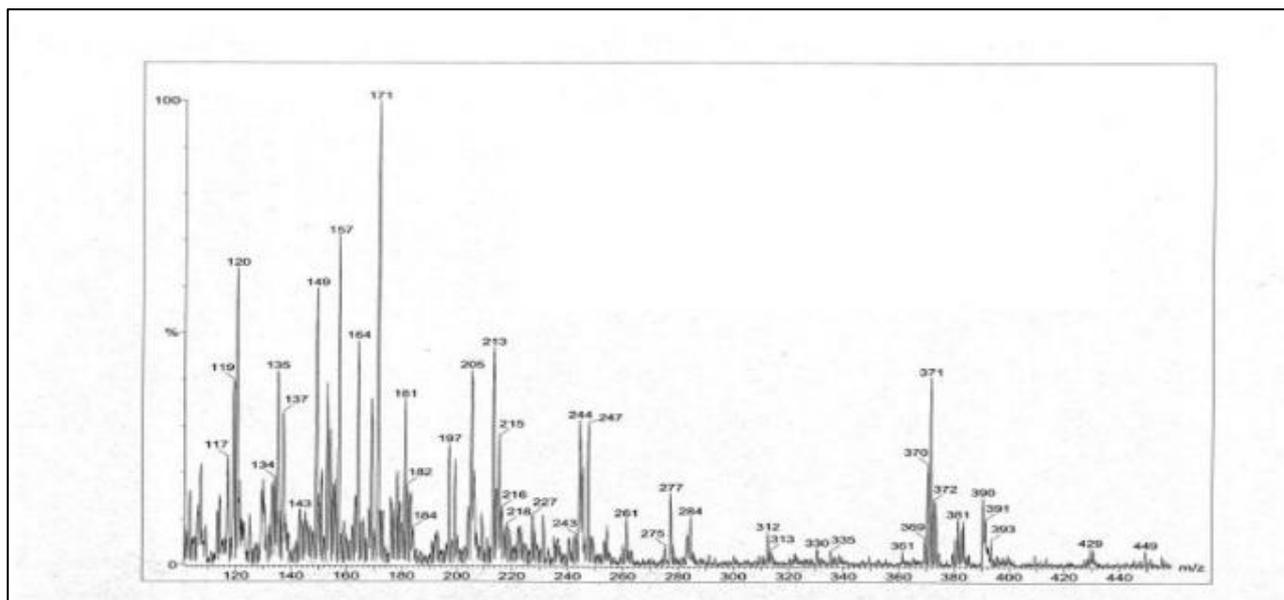


S16. FT-IR spectra of compound (3c)

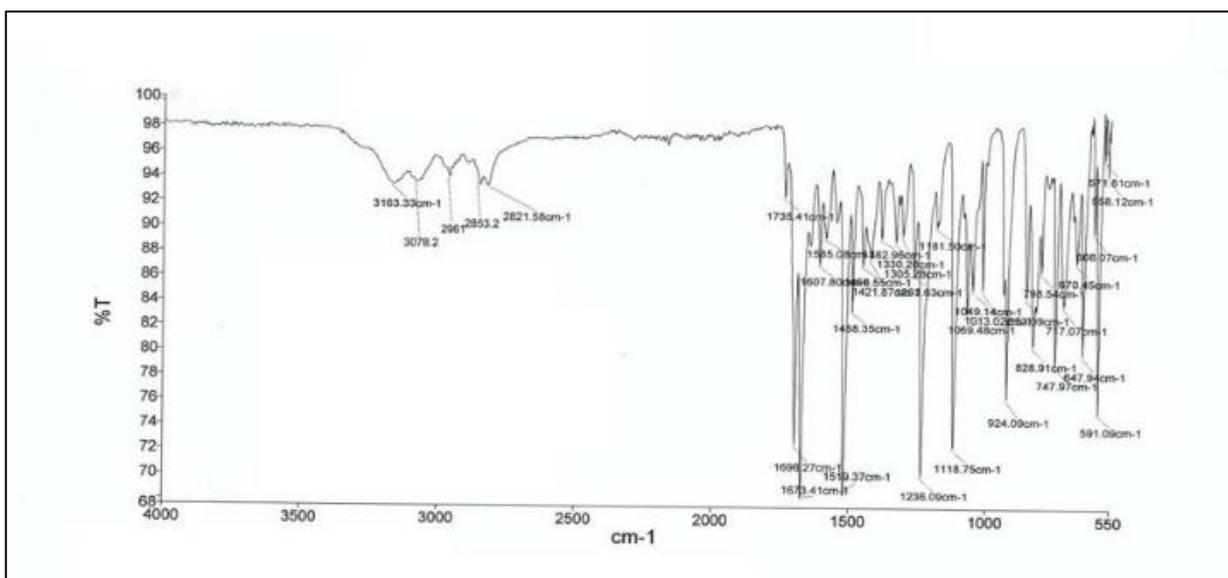
S17. ¹H NMR spectra of compound (3c)



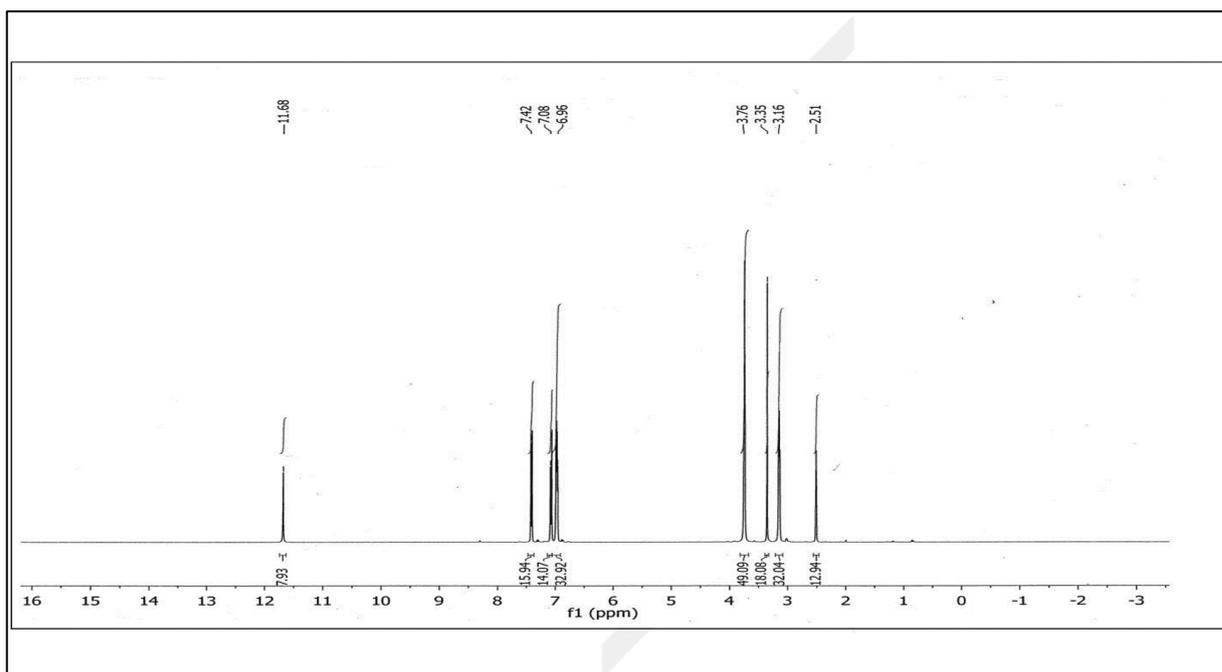
S18. ¹³C NMR (APT) spectra of compound (3c)

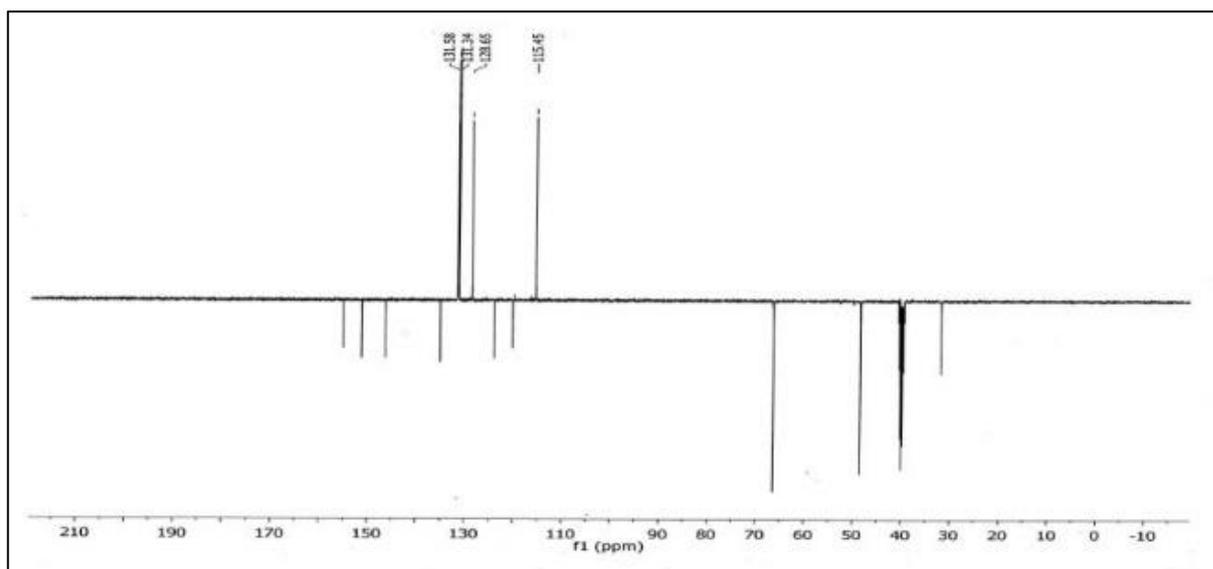
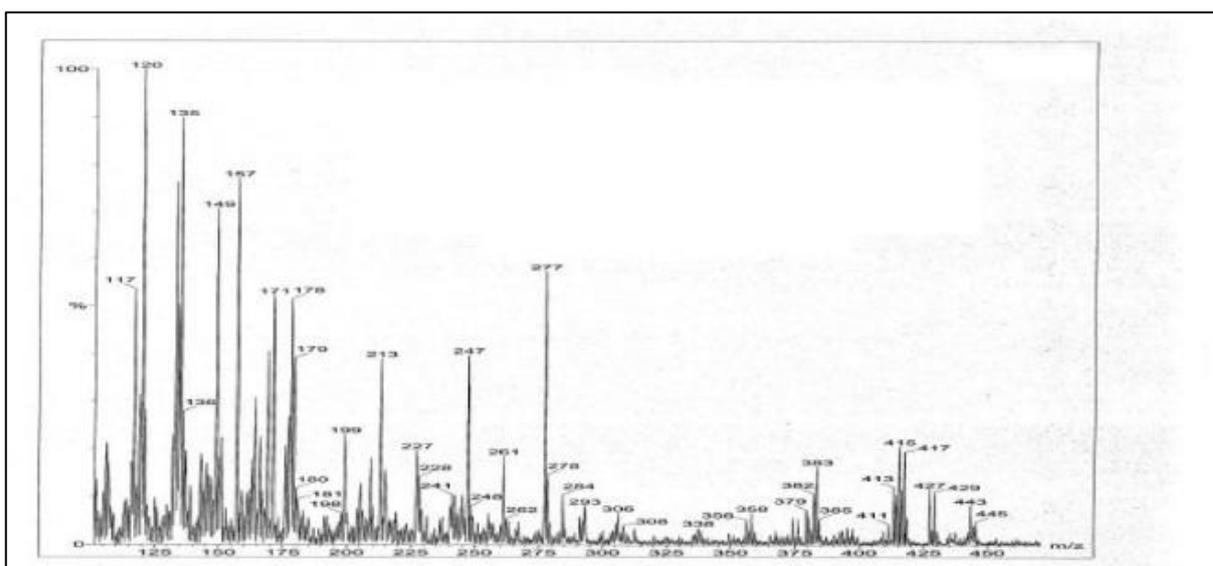


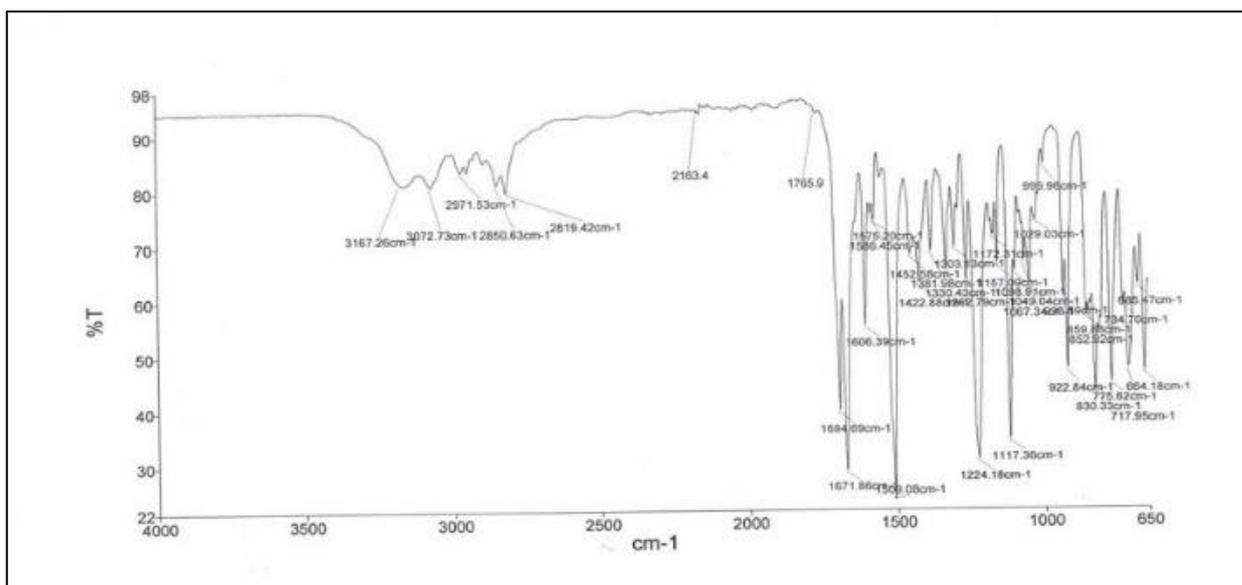
S19. Mass spectra of compound (3c)



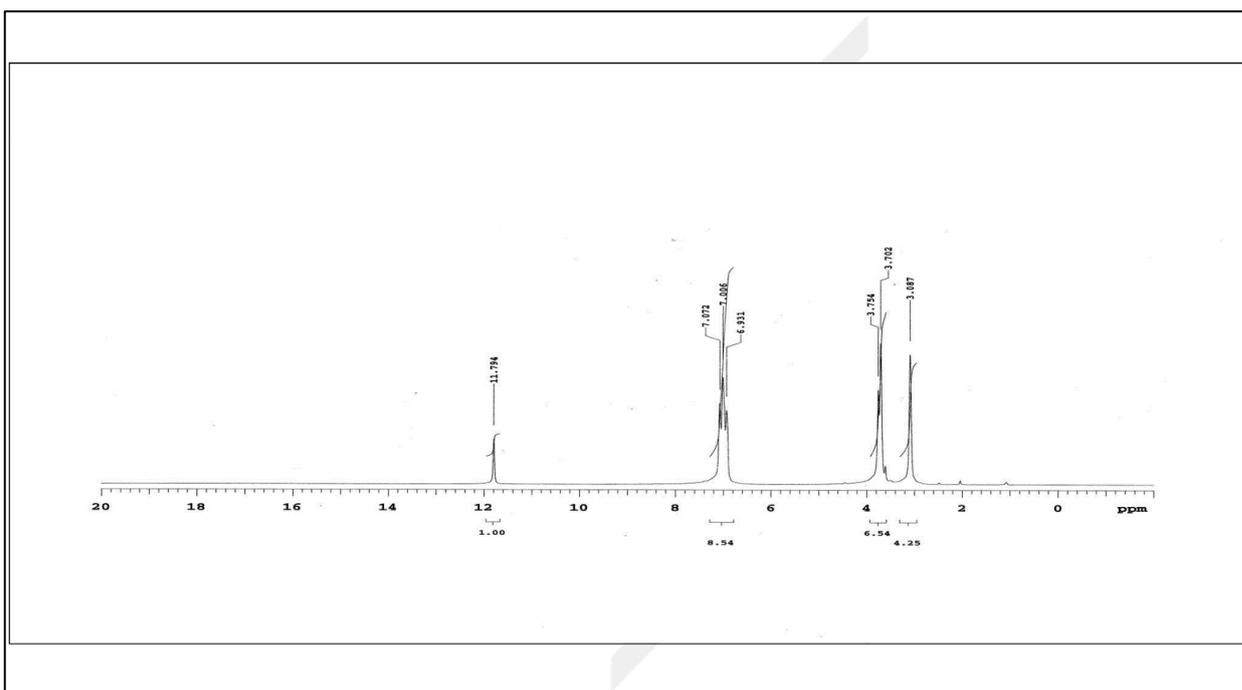
S20. FT-IR spectra of compound (3d)

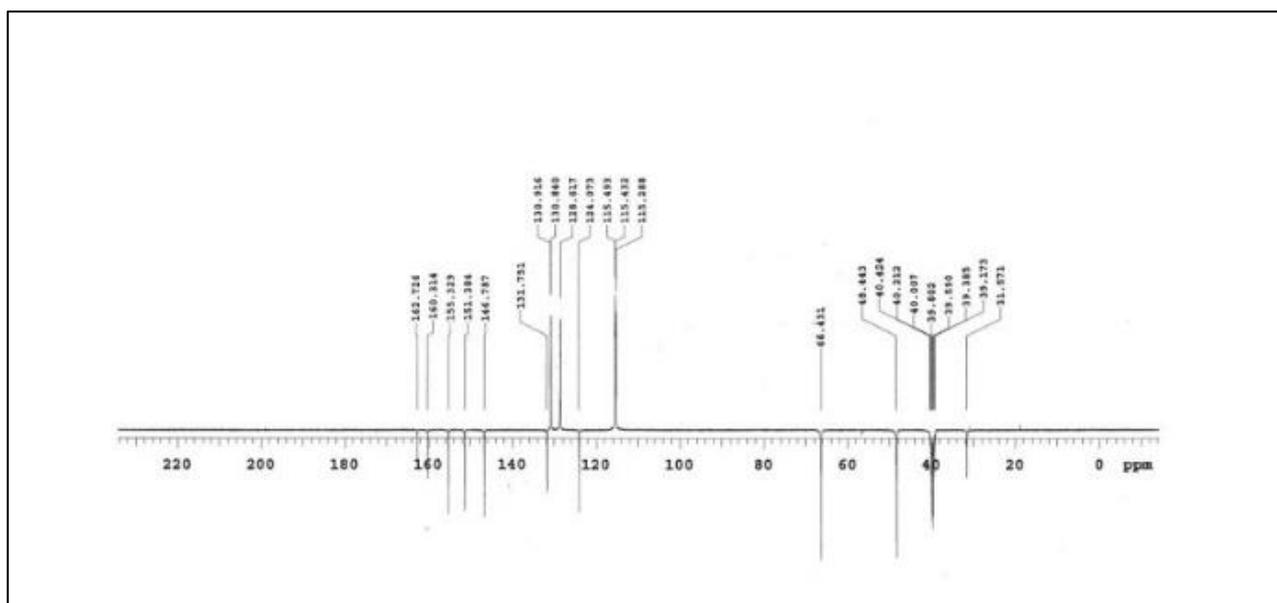
S21. ¹H NMR spectra of compound (3d)

**S22.** ¹³C NMR (APT) spectra of compound (3d)**S23.** Mass spectra of compound (3d)

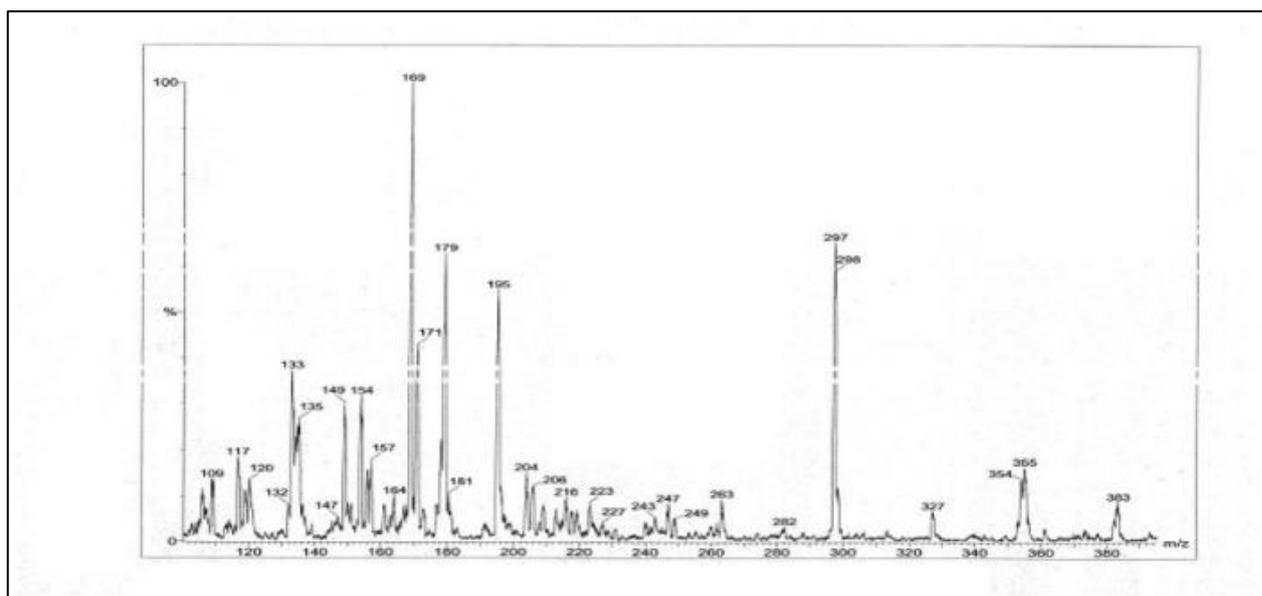


S24. FT-IR spectra of compound (3e)

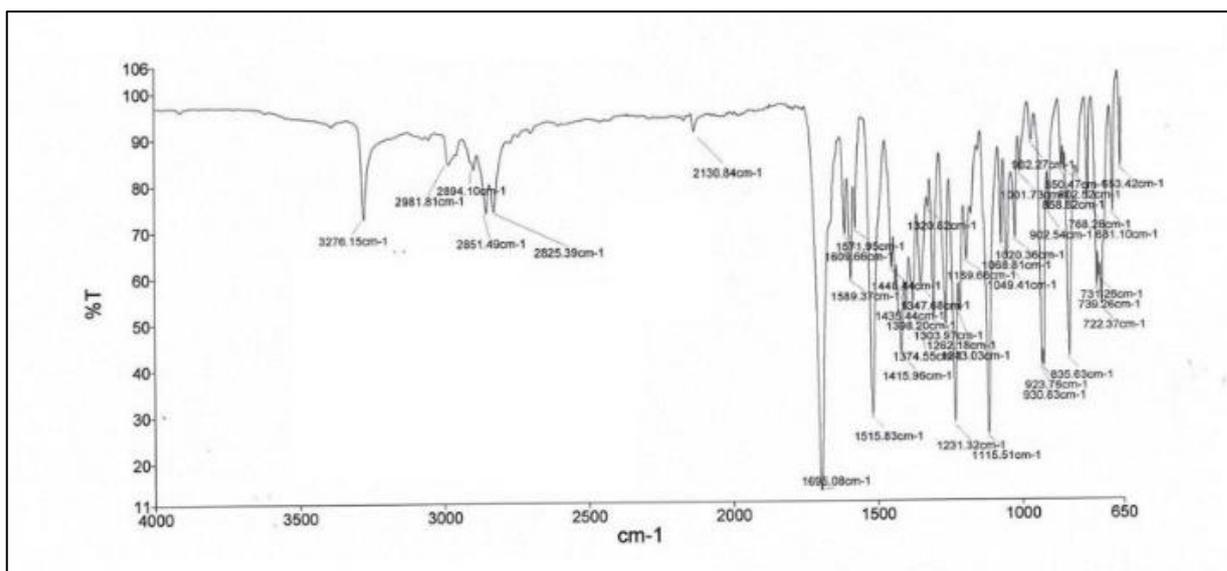
S25. ¹H NMR spectra of compound (3e)



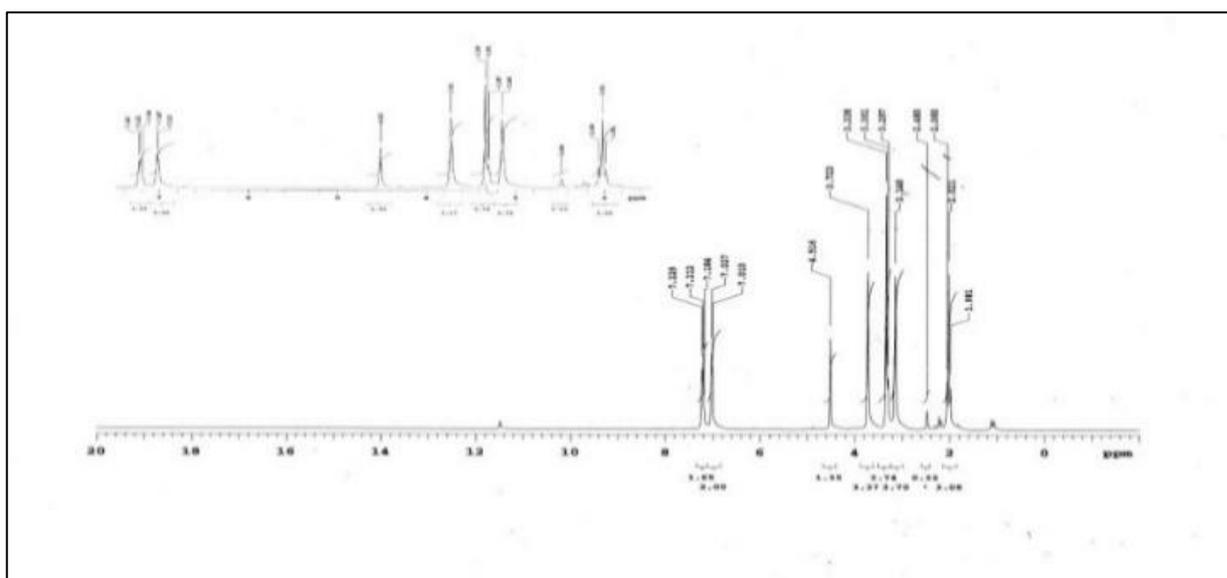
S26. ¹³C NMR (APT) spectra of compound (3e)

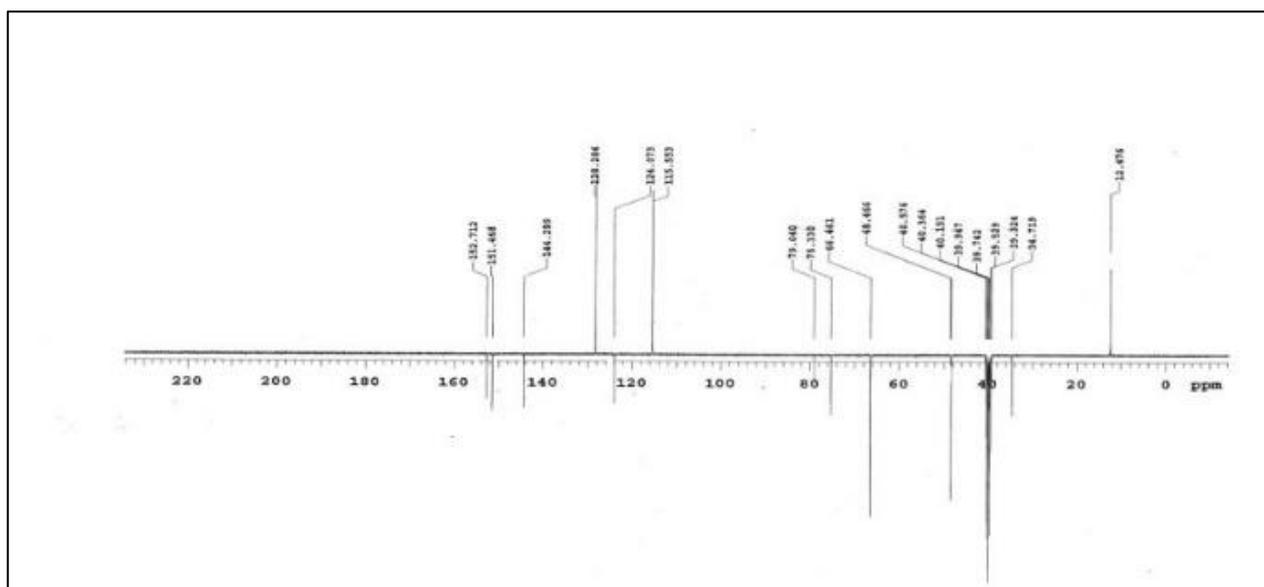


S27. Mass spectra of compound (3e)

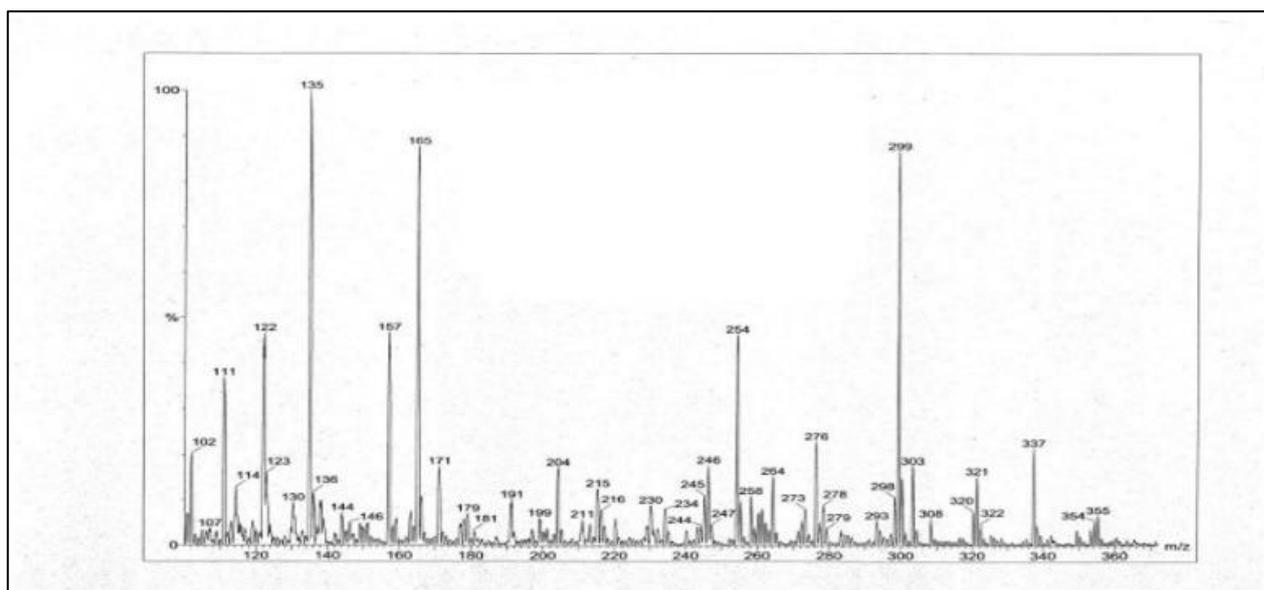


S28. FT-IR spectra of compound (4a)

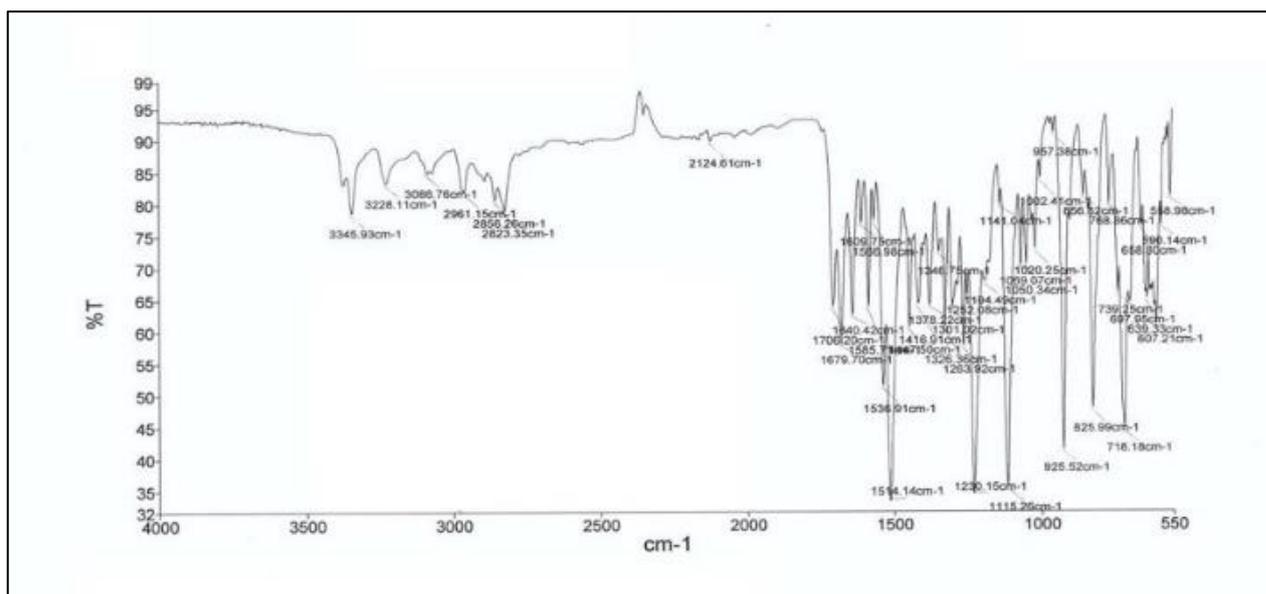
S29. ^1H NMR spectra of compound (4a)



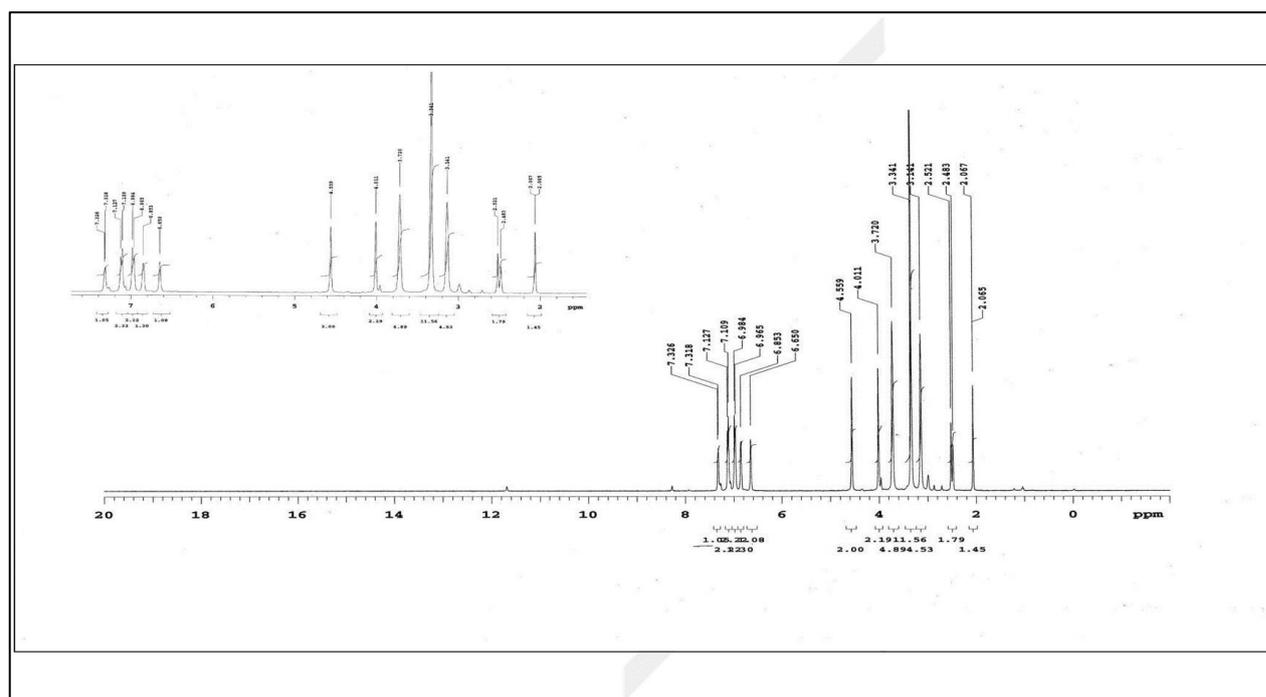
S30. ¹³C NMR (APT) spectra of compound (4a)

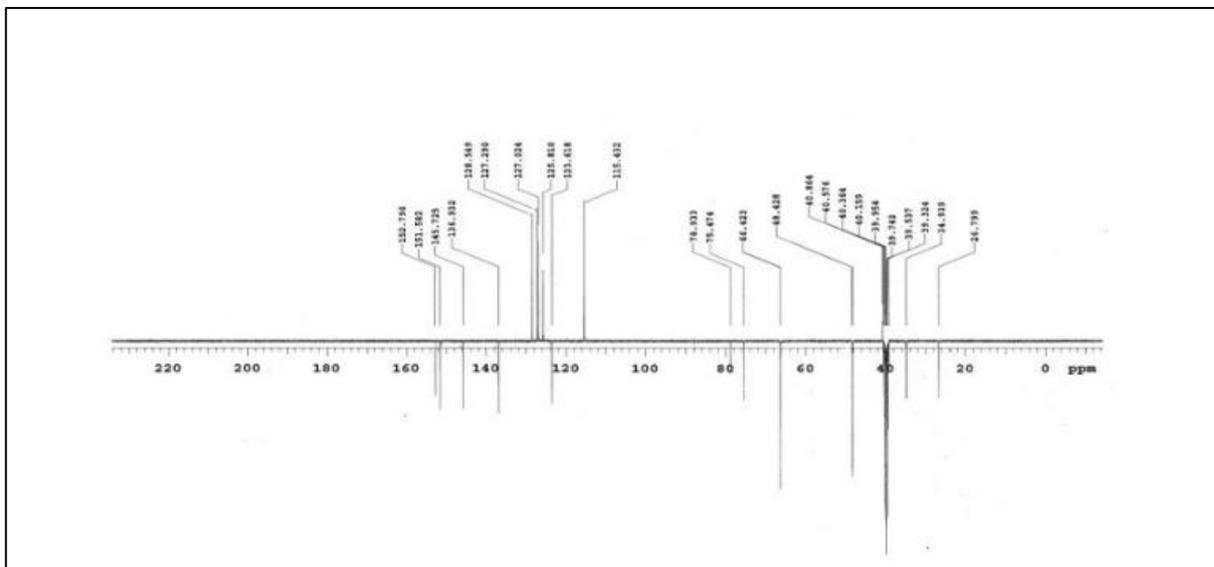


S31. Mass spectra of compound (4a)

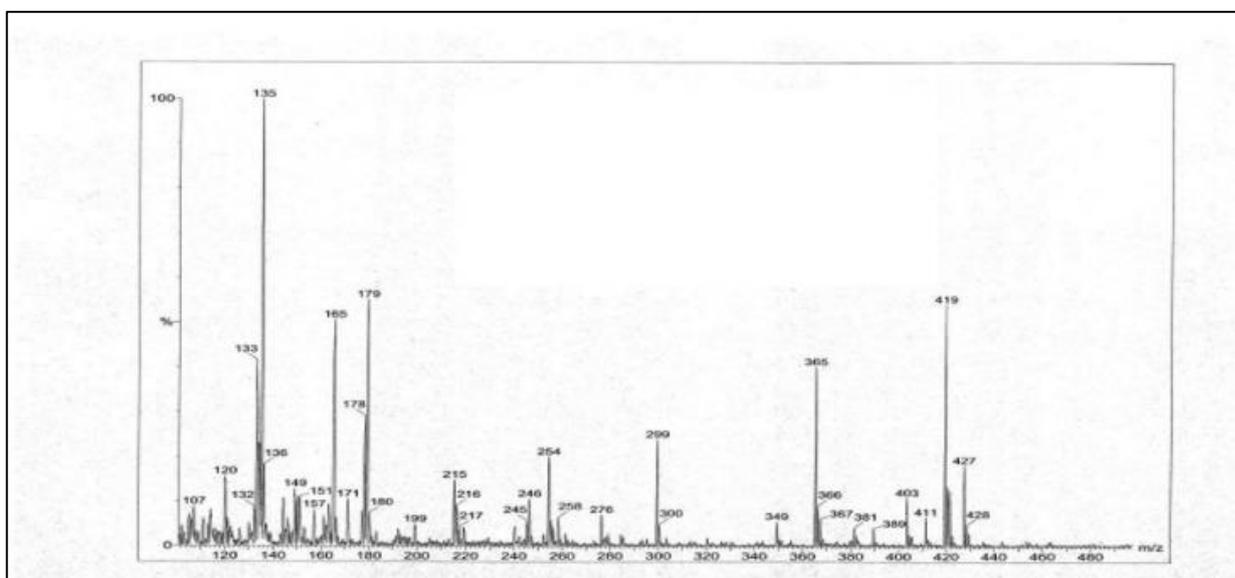


S32. FT-IR spectra of compound (4b)

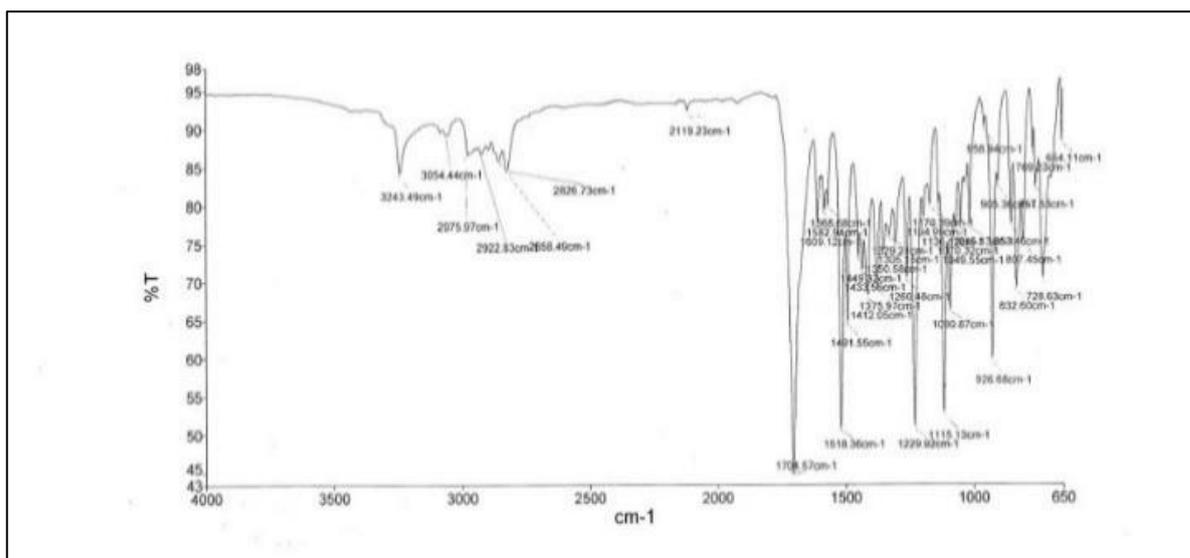
S33. ¹H NMR spectra of compound (4b)



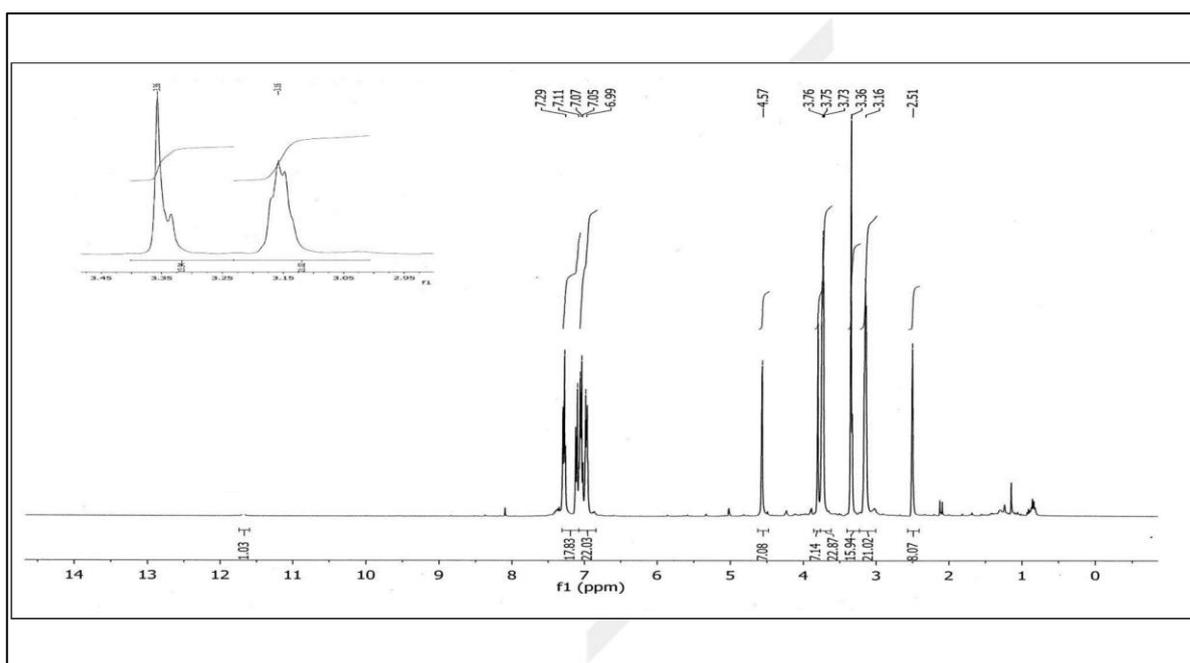
S34. ^{13}C NMR (APT) spectra of compound (4b)

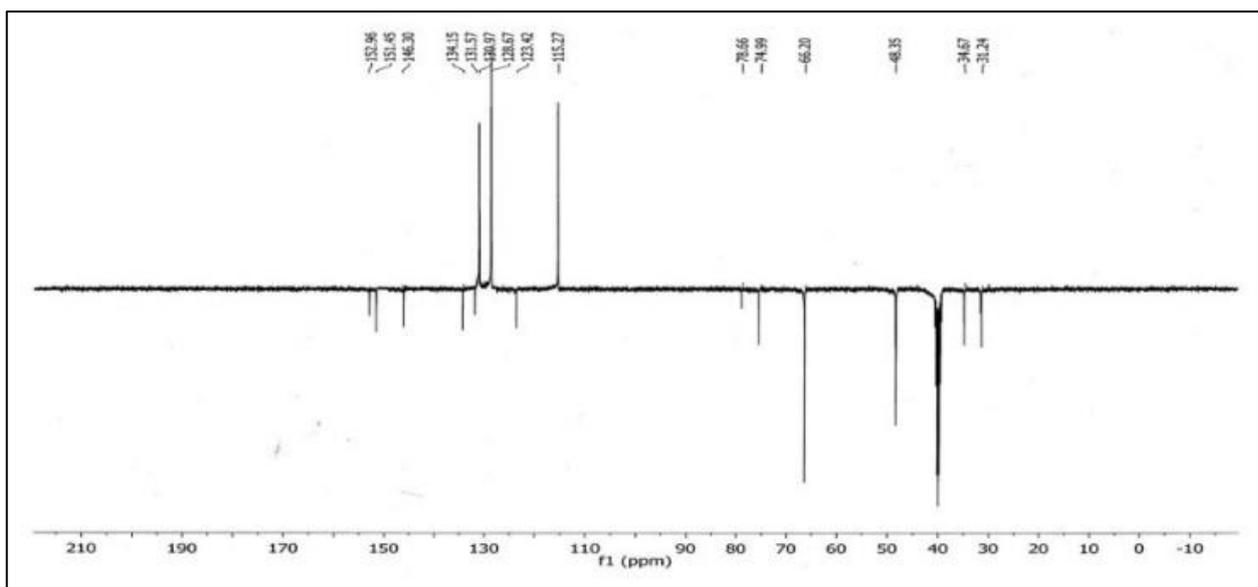


S35. Mass spectra of compound (4b)

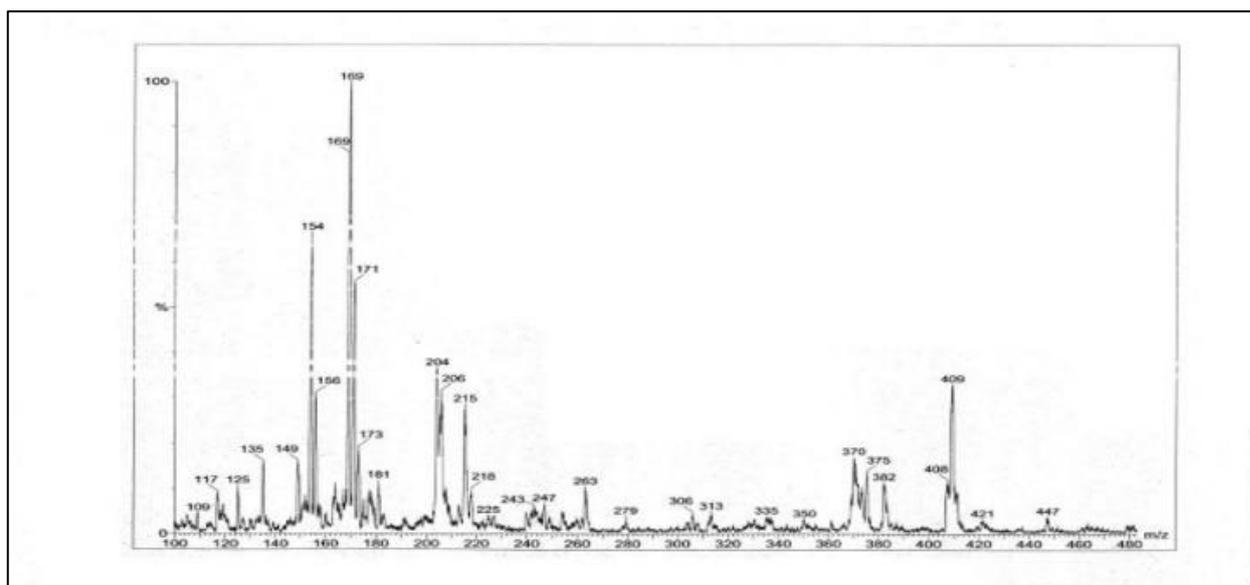


S36. FT-IR spectra of compound (4c)

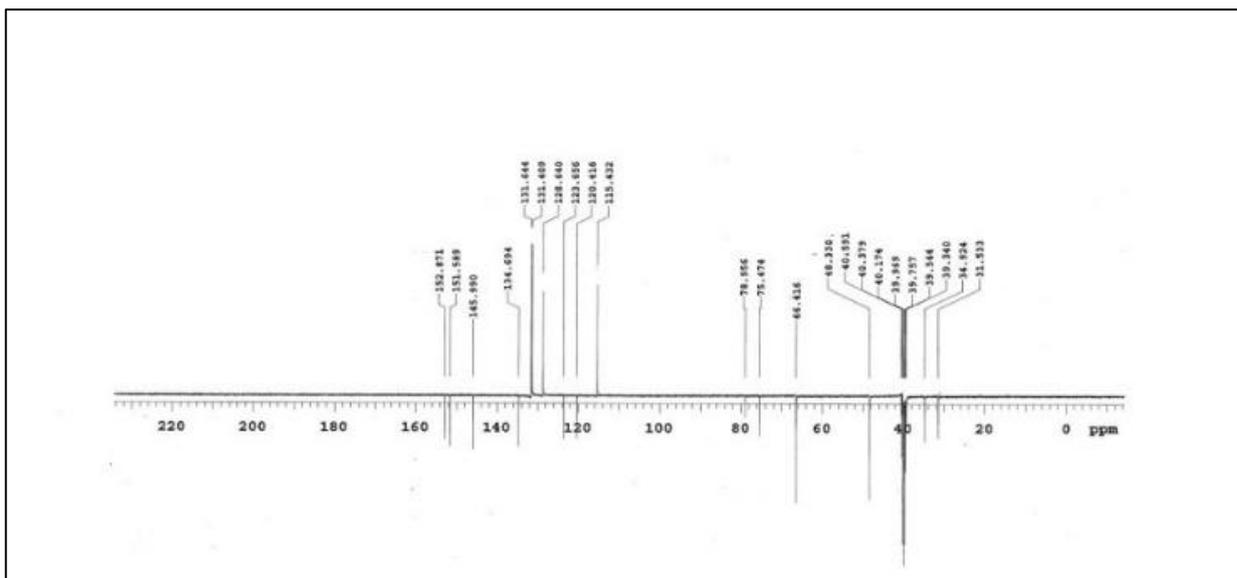
S37. ¹H NMR spectra of compound (4c)



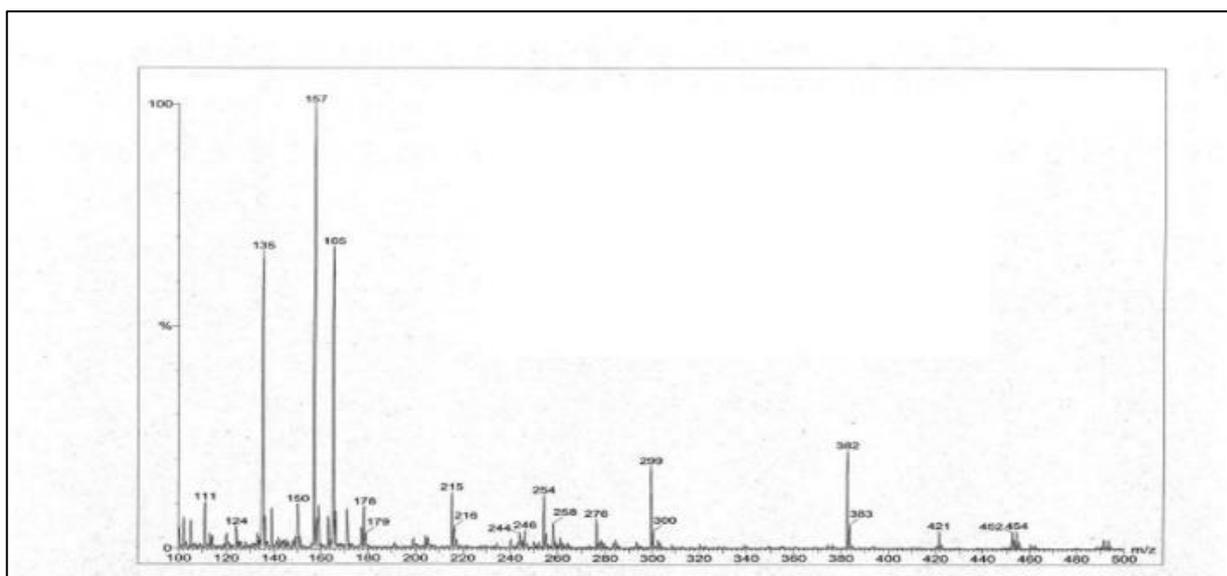
S38. ¹³C NMR (APT) spectra of compound (4c)



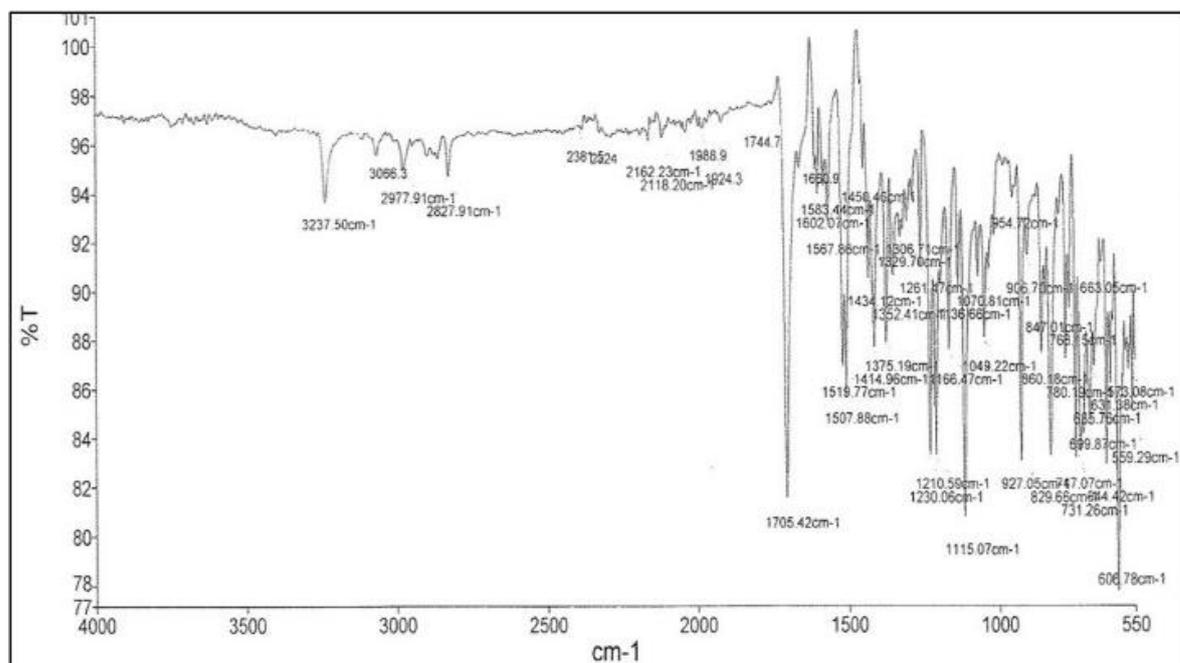
S39. Mass spectra of compound (4c)



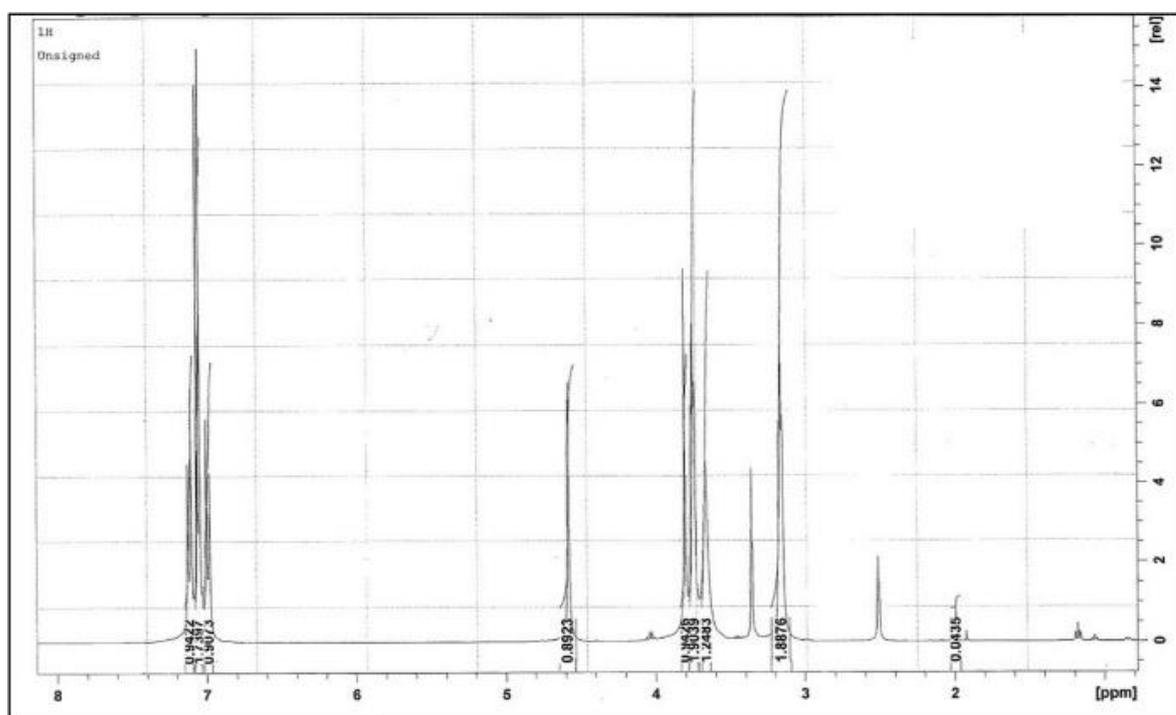
S42. ¹³C NMR (APT) spectra of compound (4d)

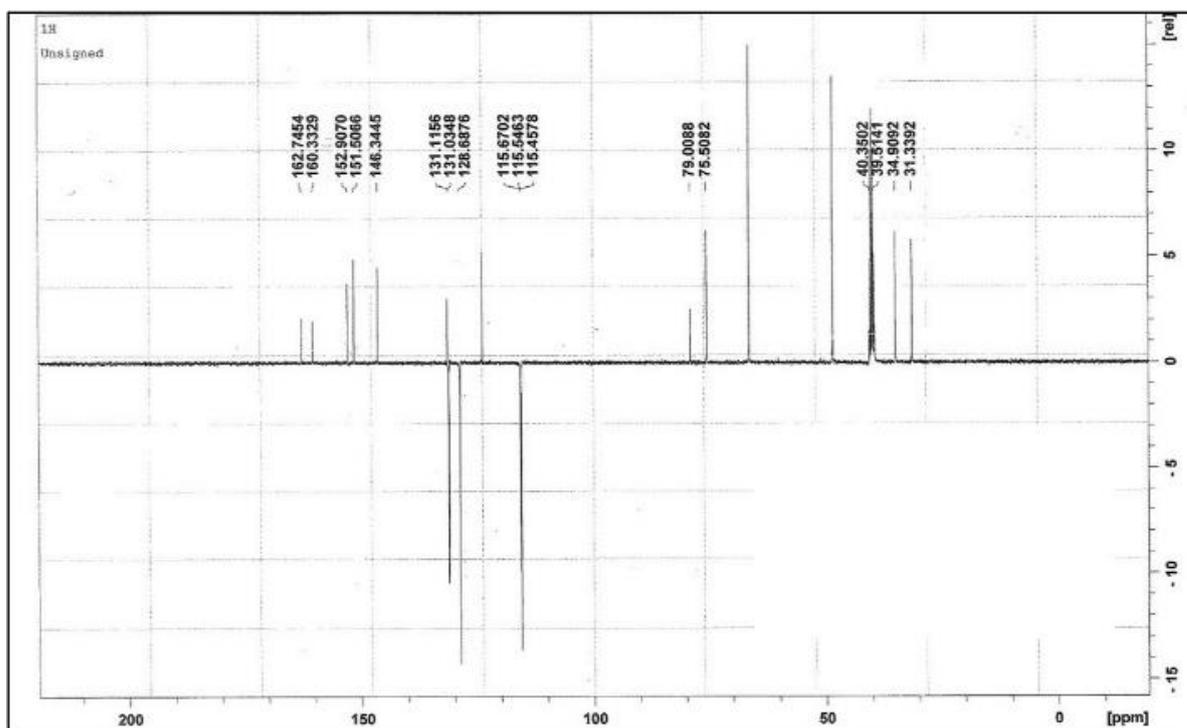


S43. Mass spectra of compound (4d)

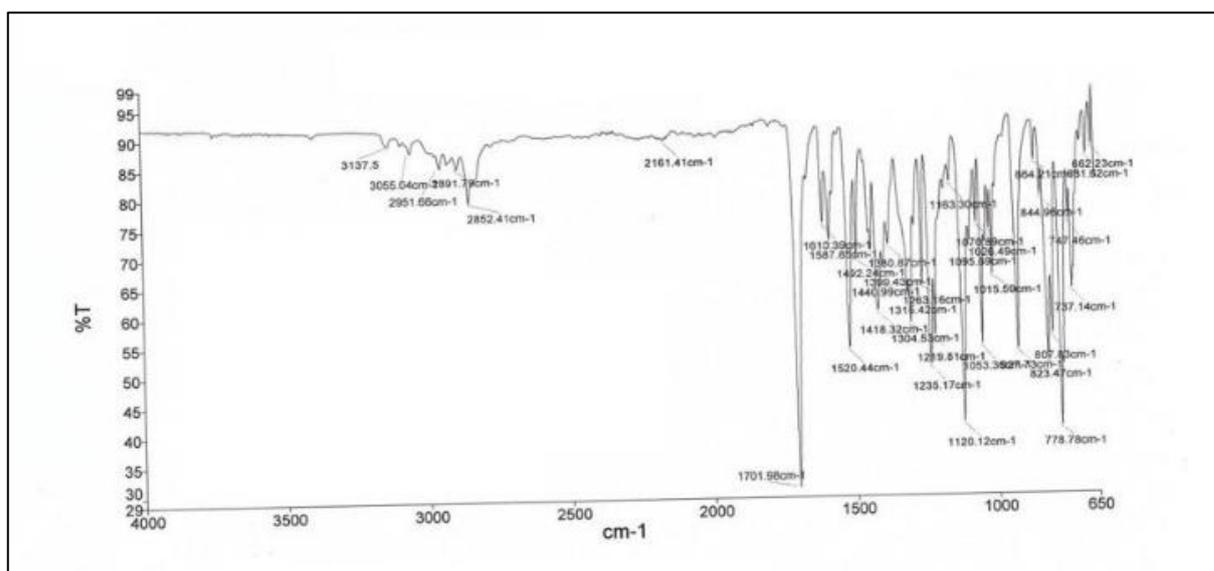


S44. FT-IR spectra of compound (4e)

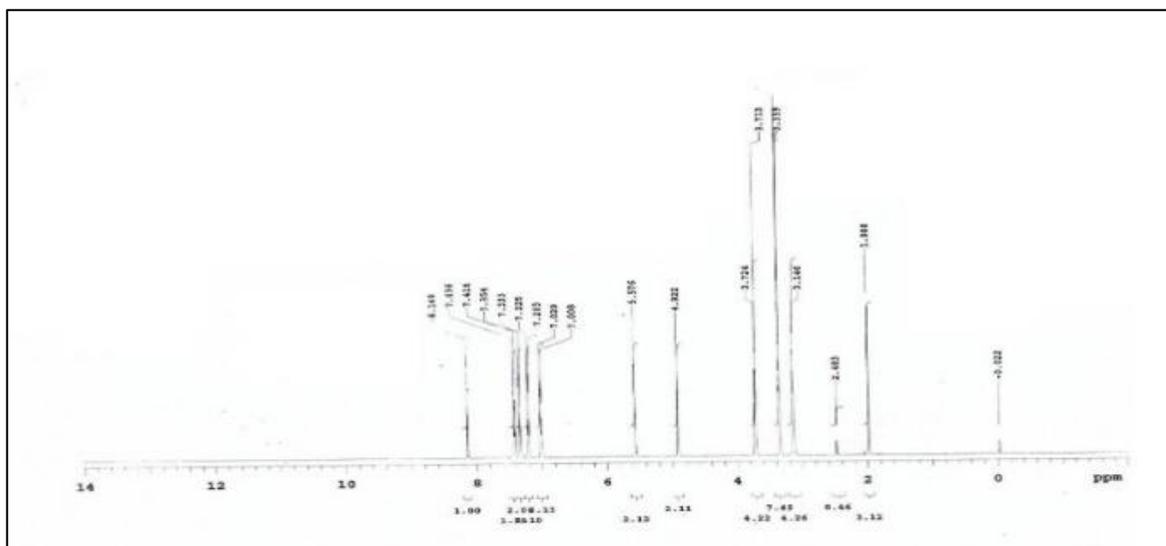
S45. ¹H NMR spectra of compound (4e)



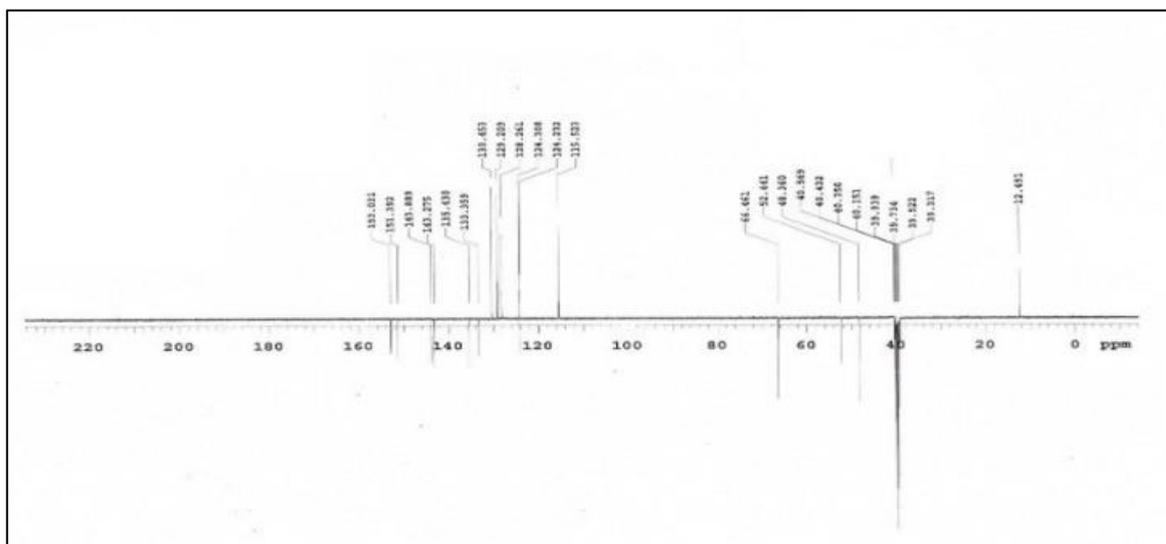
S46. ^{13}C NMR (APT) spectra of compound (4e)



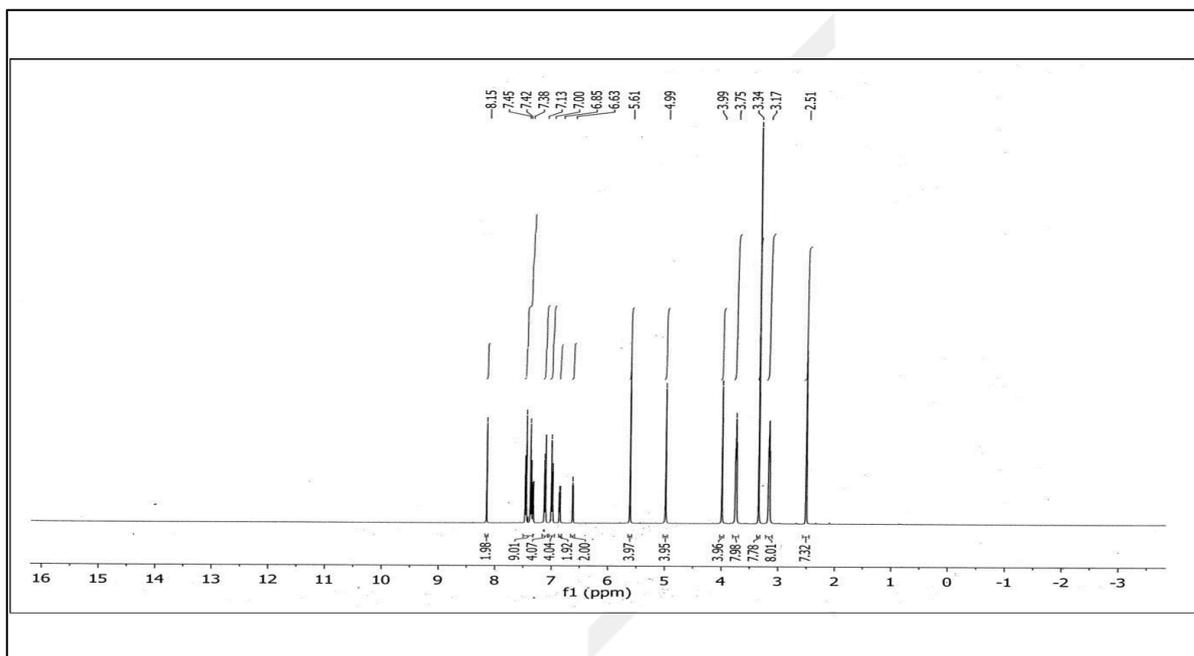
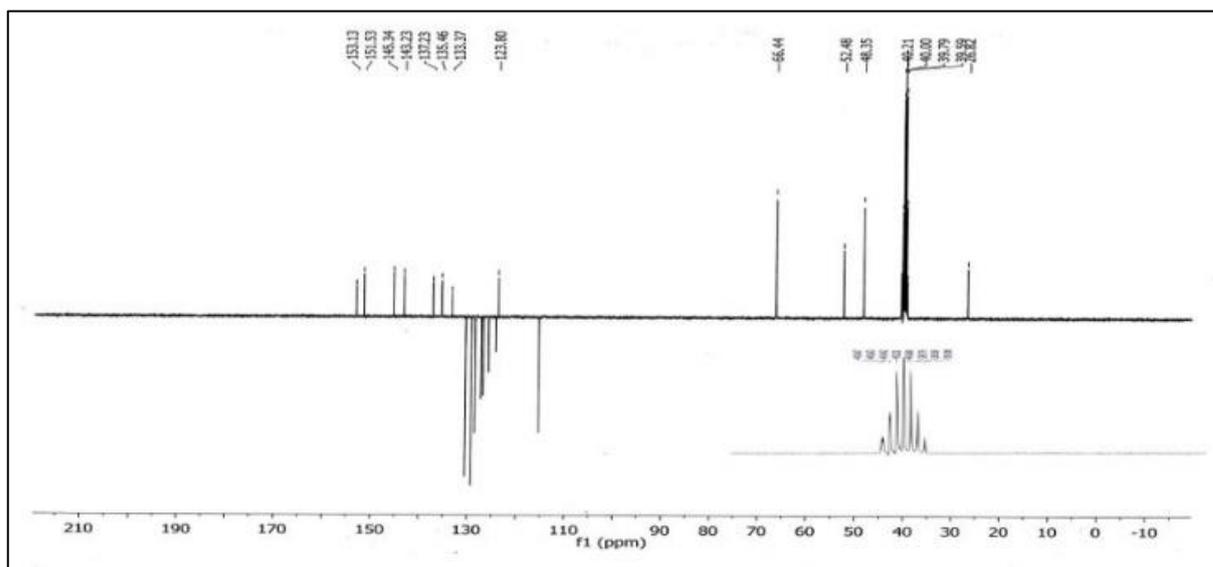
S47. FT-IR spectra of compound (5a)

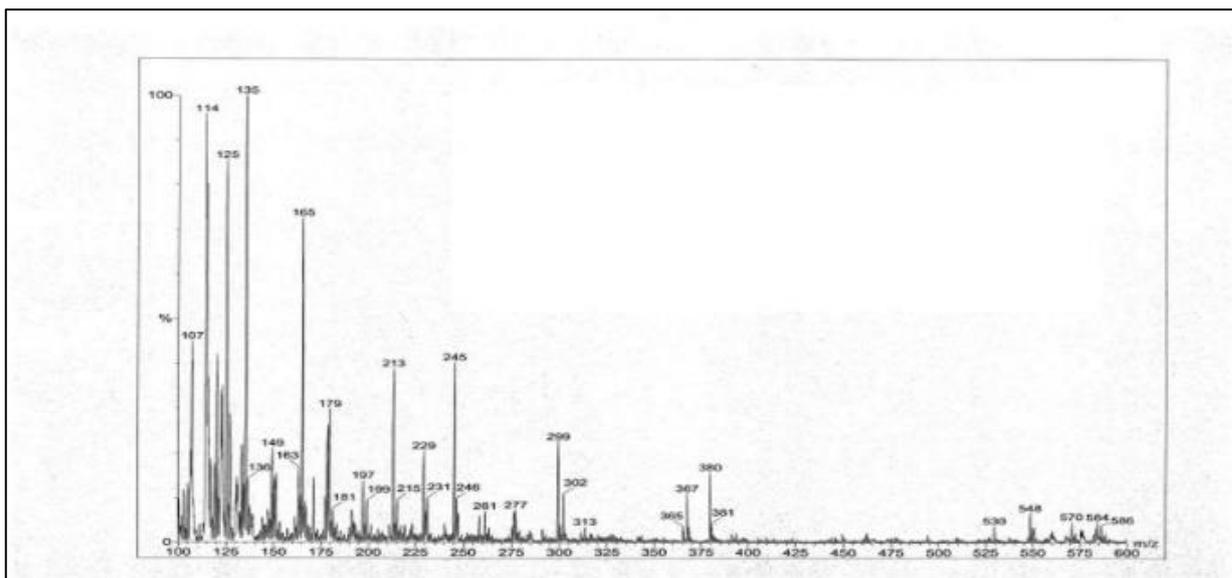


S48. ¹H NMR spectra of compound (5a)

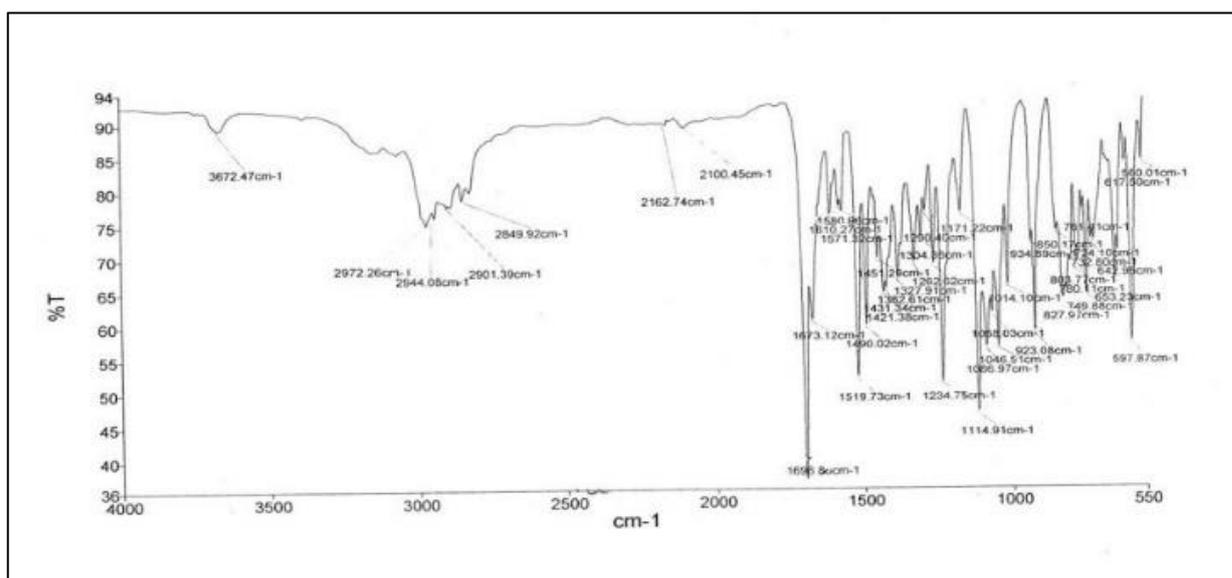


S49. ¹³C NMR (APT) spectra of compound (5a)

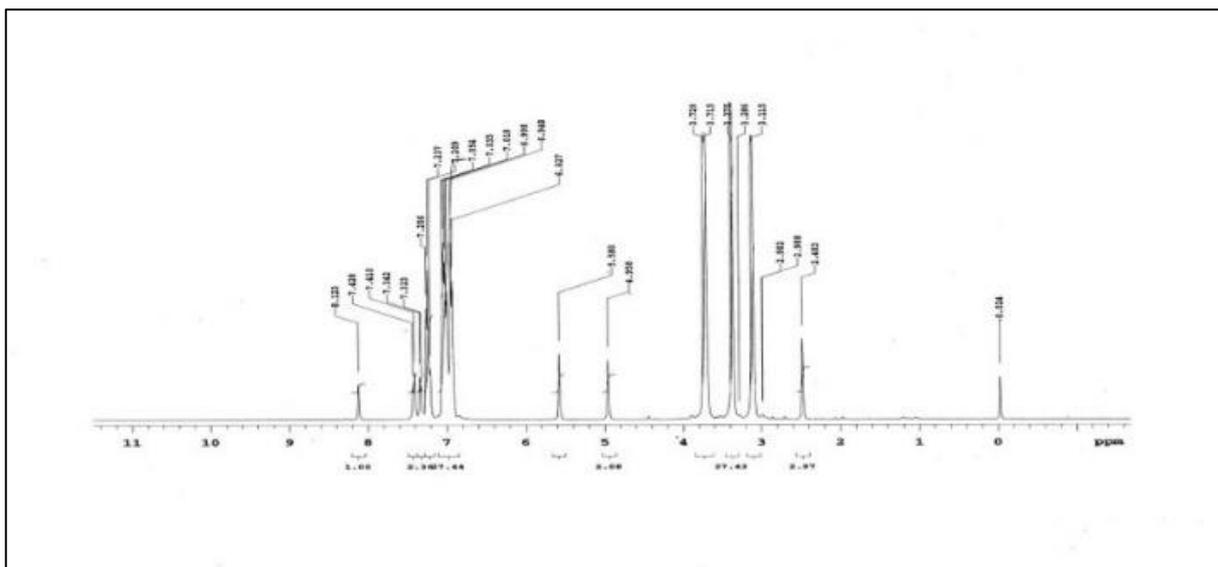
S52. ¹H NMR spectra of compound (5b)S53. ¹³C NMR (APT) spectra of compound (5b)



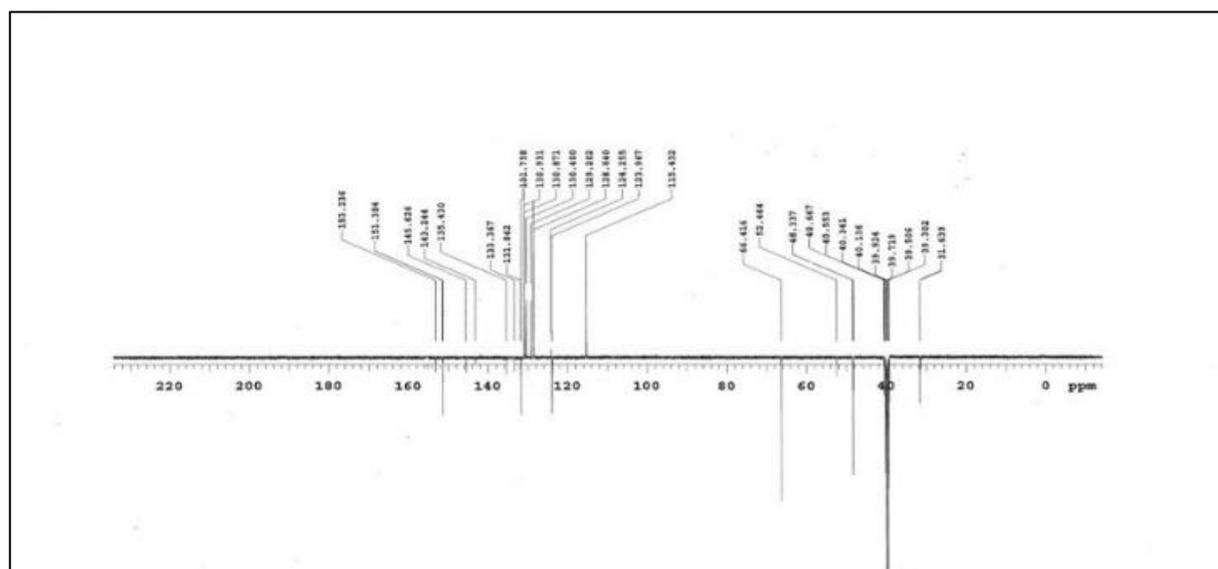
S54. Mass spectra of compound (5b)



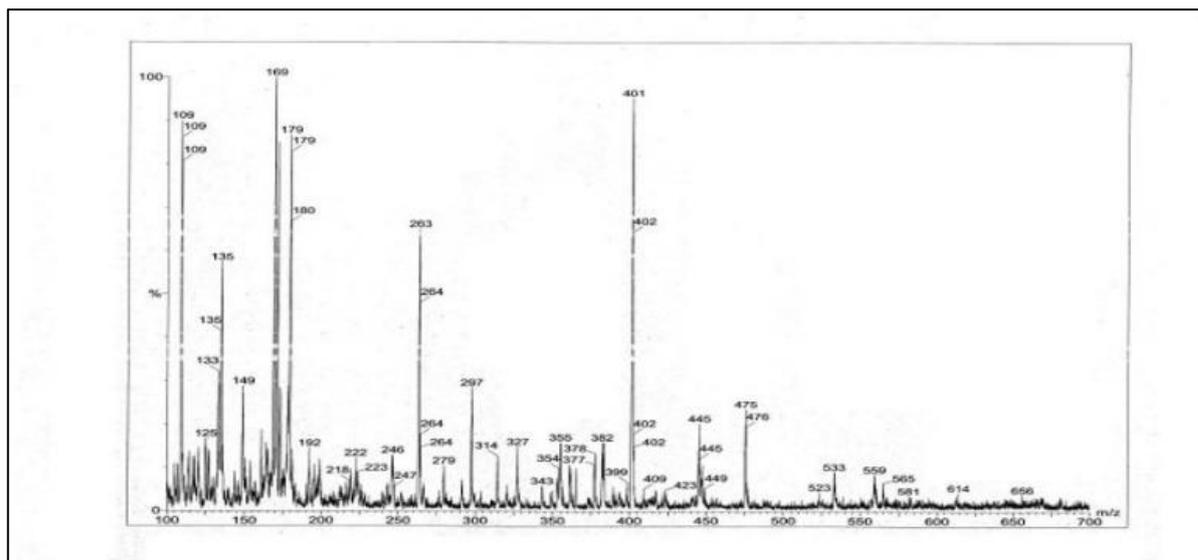
S55. FT-IR spectra of compound (5c)



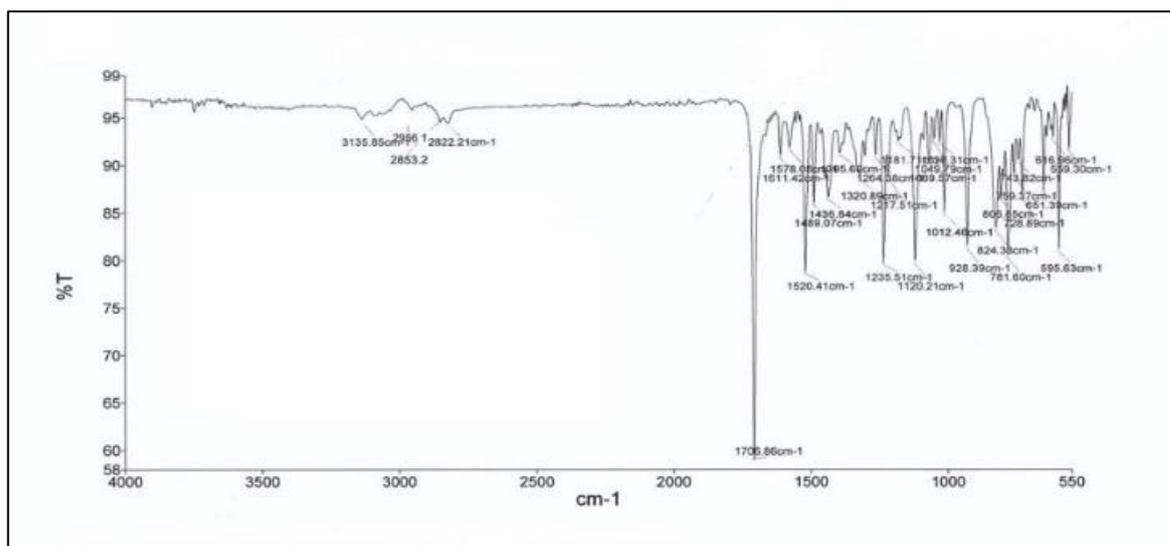
S56. ¹H NMR spectra of compound (5c)



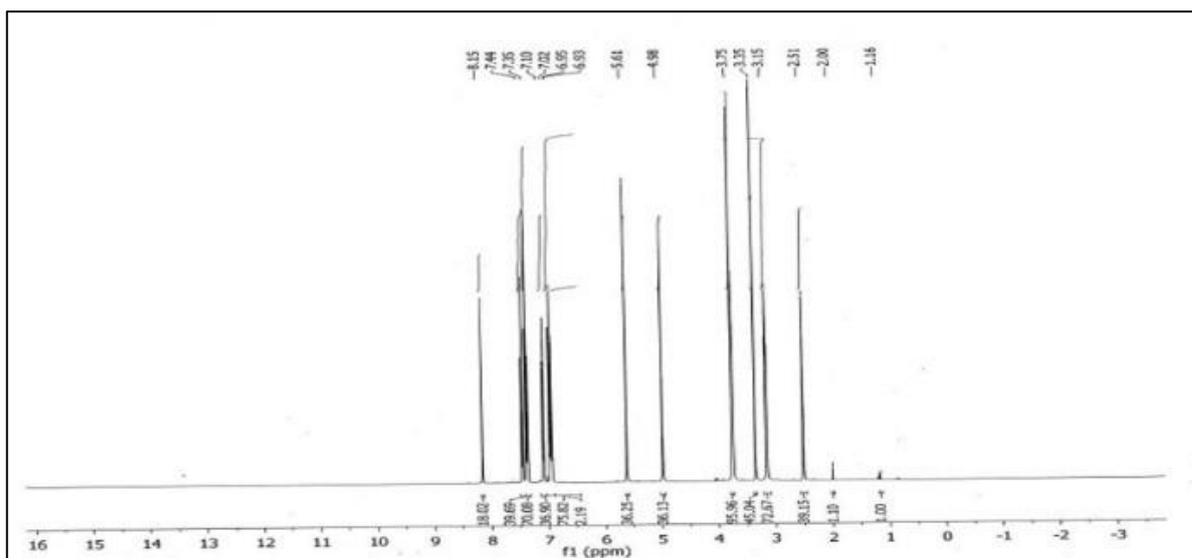
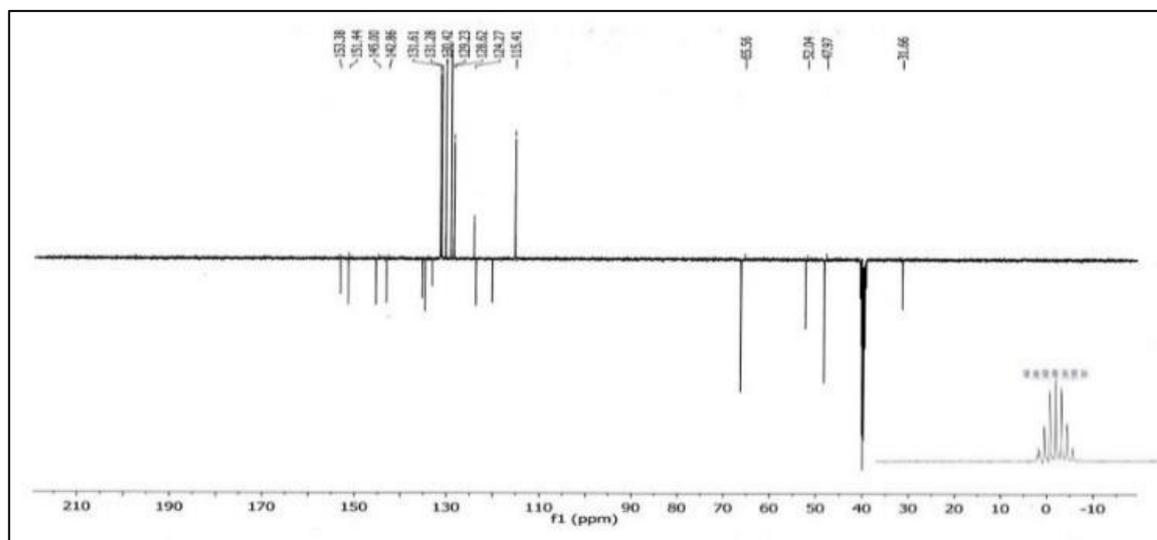
S57. ¹³C NMR (APT) spectra of compound (5c)

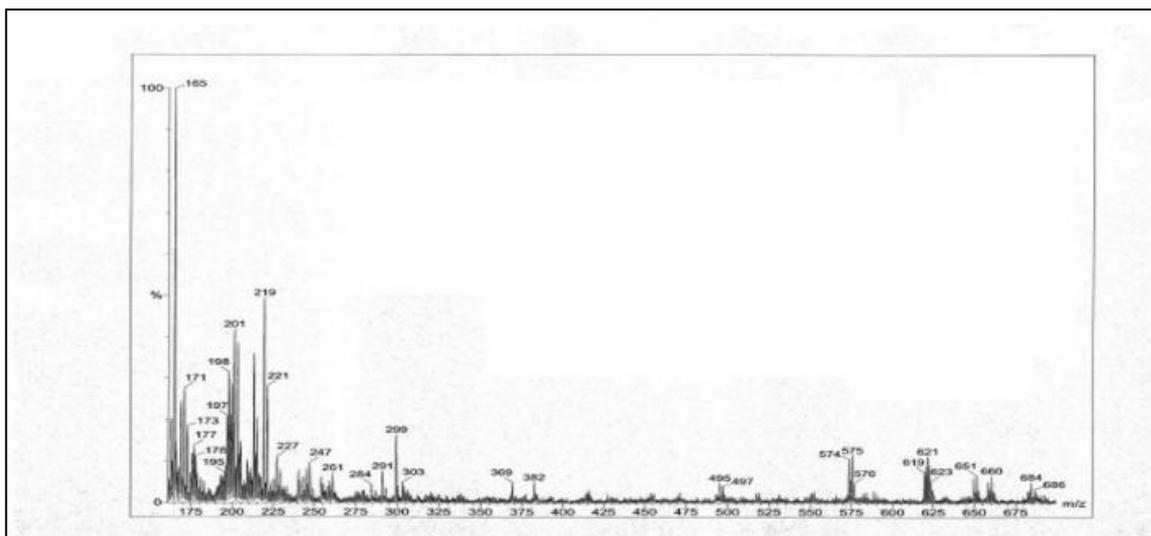


S58. Mass spectra of compound (5c)

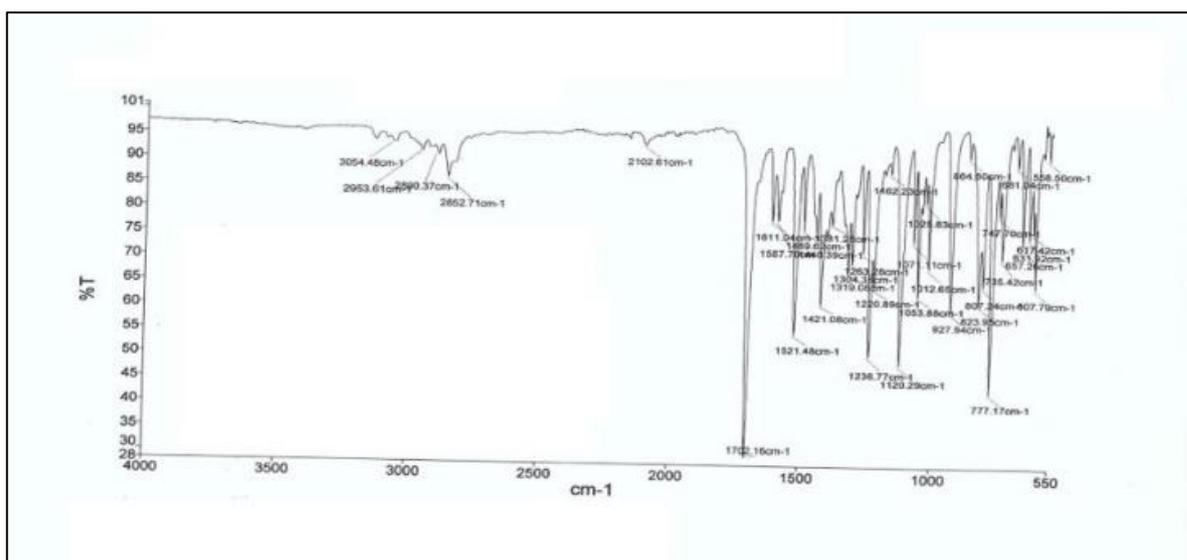


S59. FT-IR spectra of compound (5d)

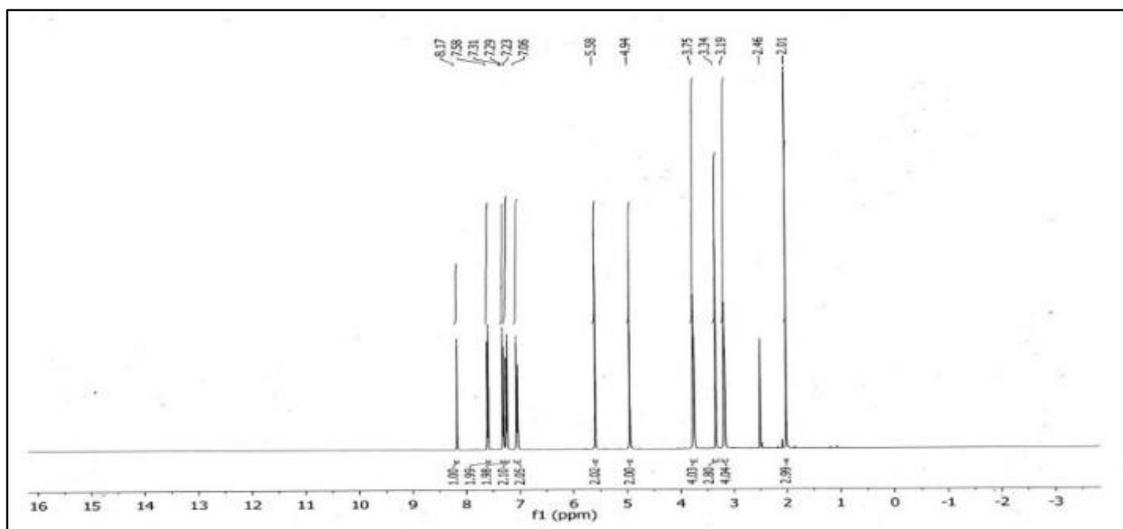
**S60.** ¹H NMR spectra of compound (5d)**S61.** ¹³C NMR (APT) spectra of compound (5d)



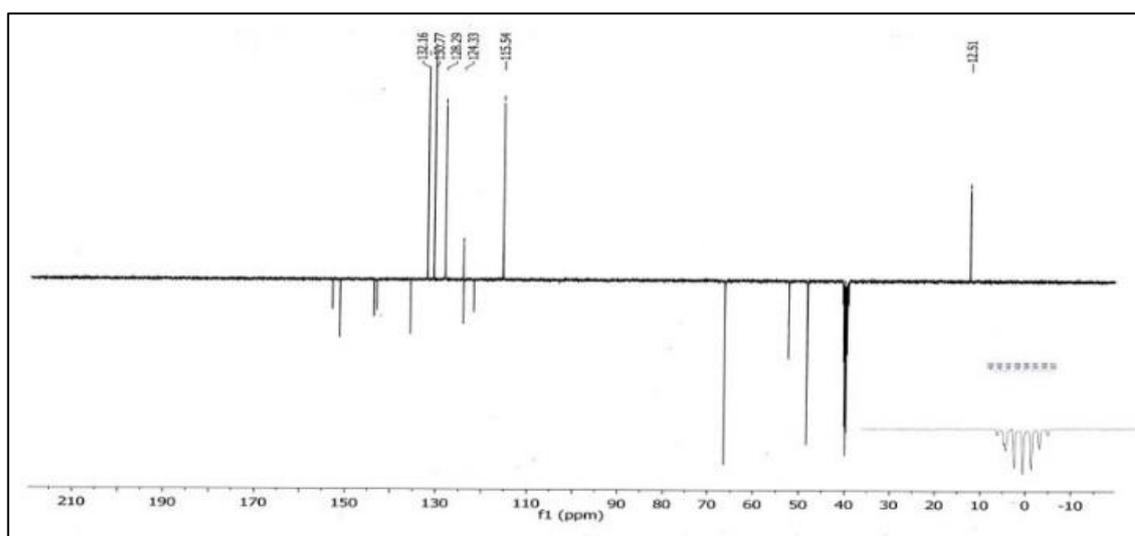
S62. Mass spectra of compound (5d)



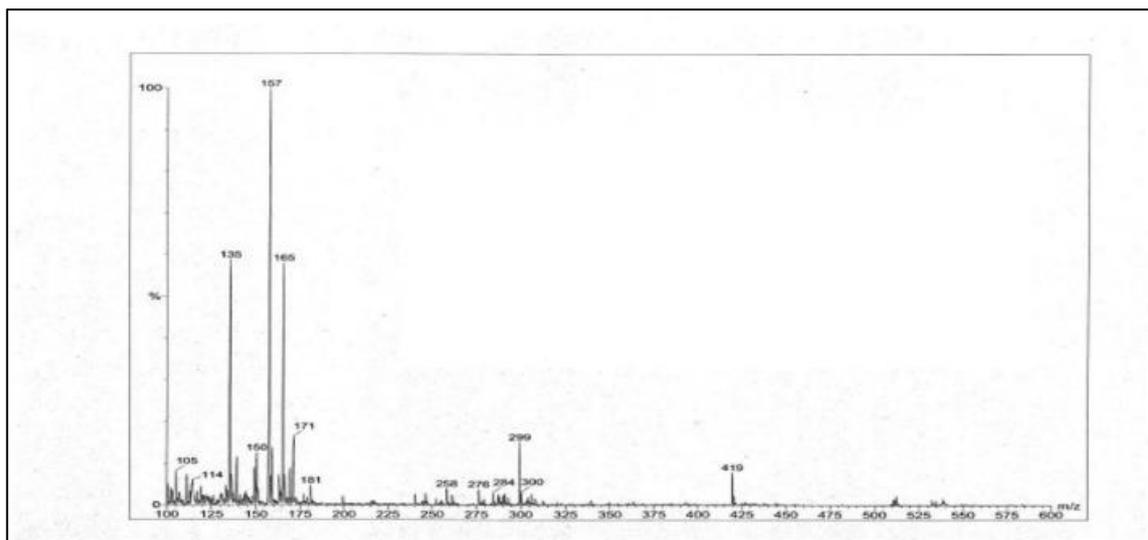
S63. FT-IR spectra of compound (6a)



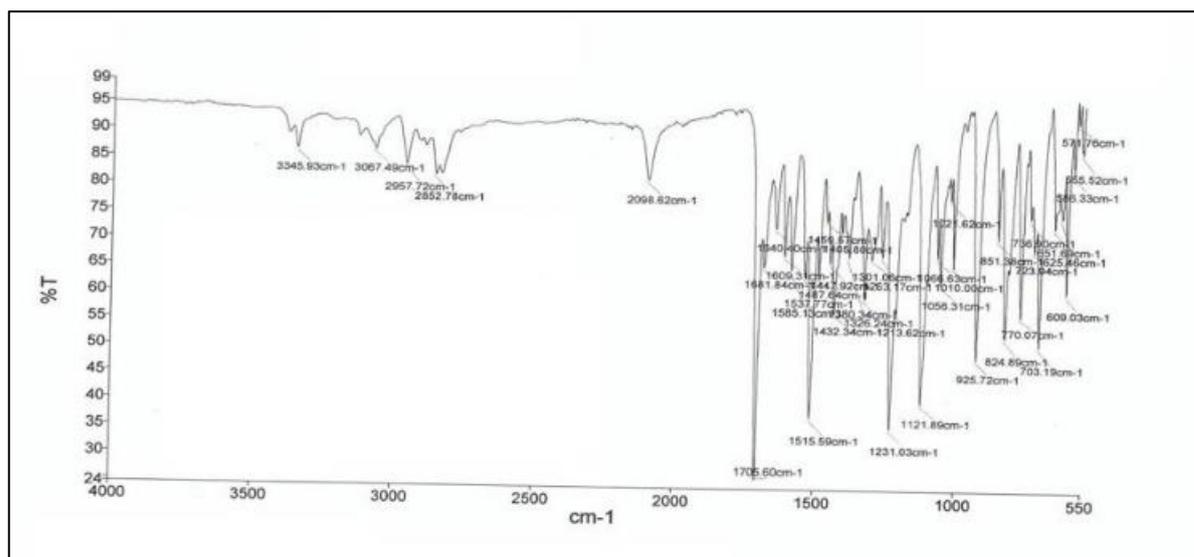
S64. ¹H NMR spectra of compound (6a)



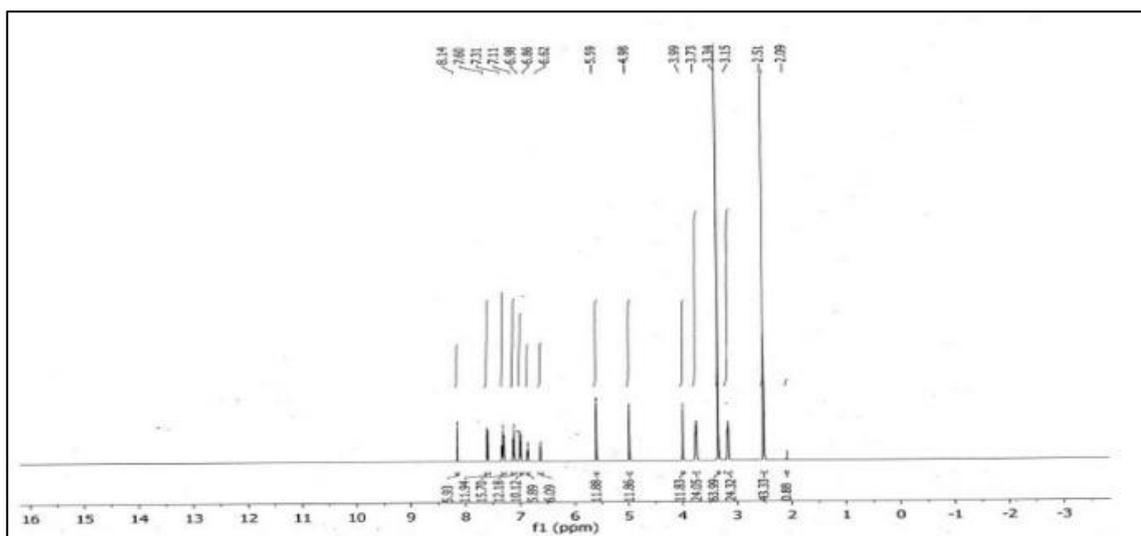
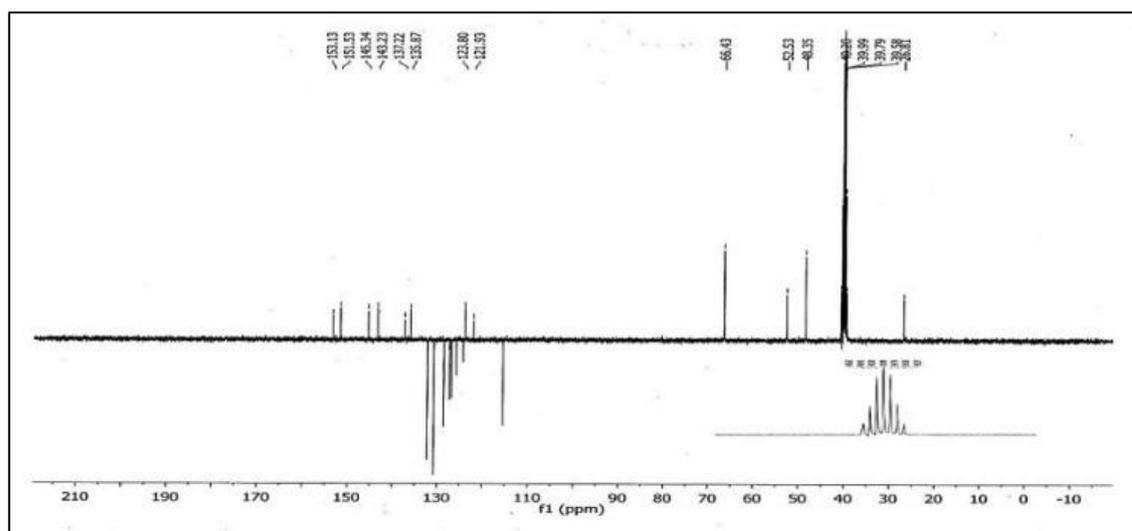
S65. ¹³C NMR (APT) spectra of compound (6a)

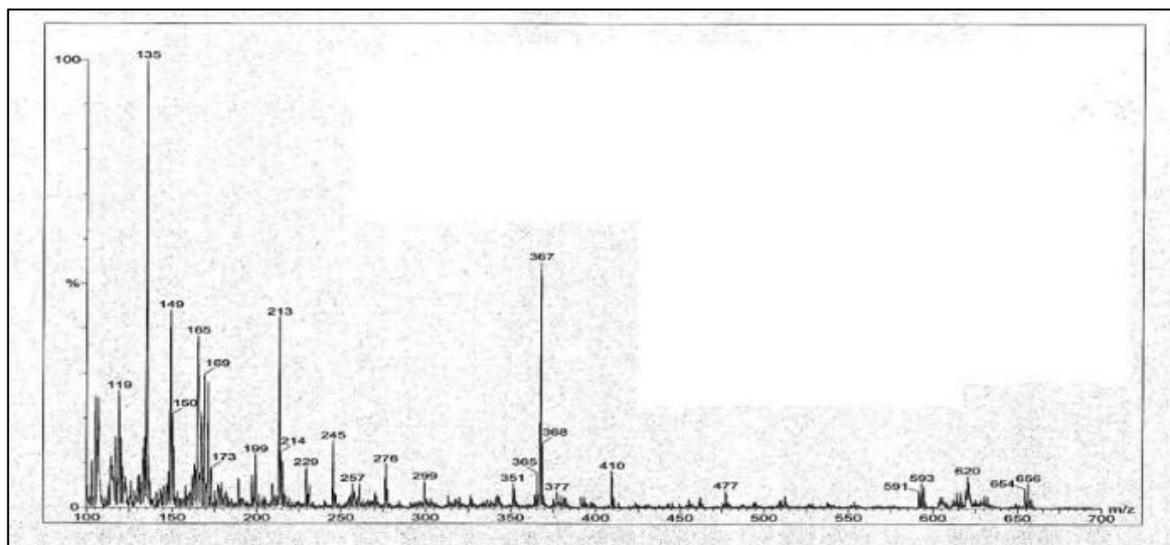


S66. Mass spectra of compound (6a)

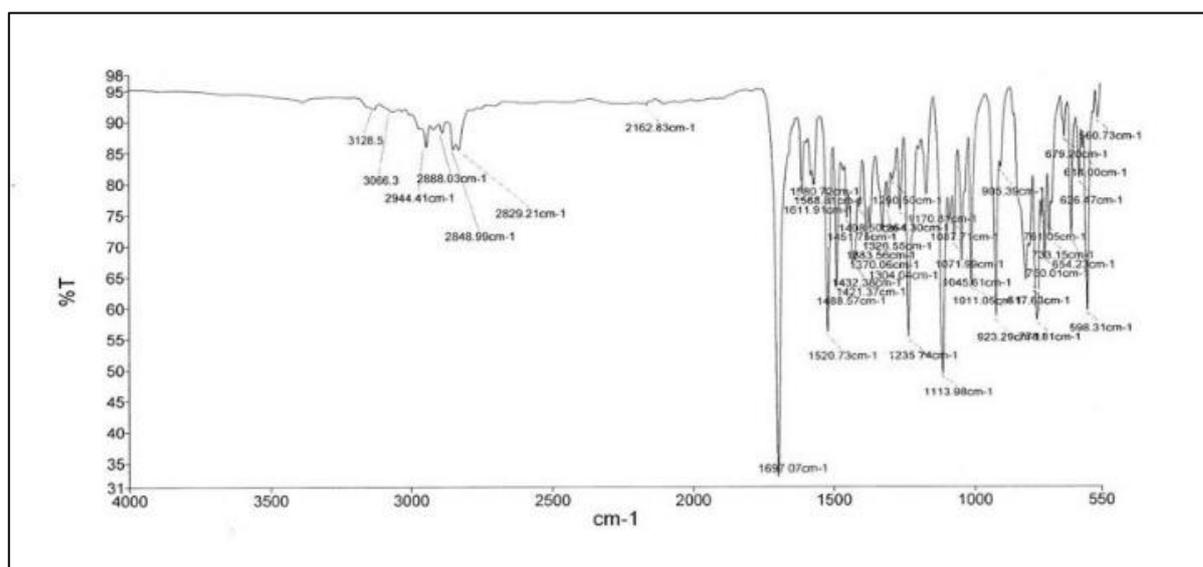


S67. FT-IR spectra of compound (6b)

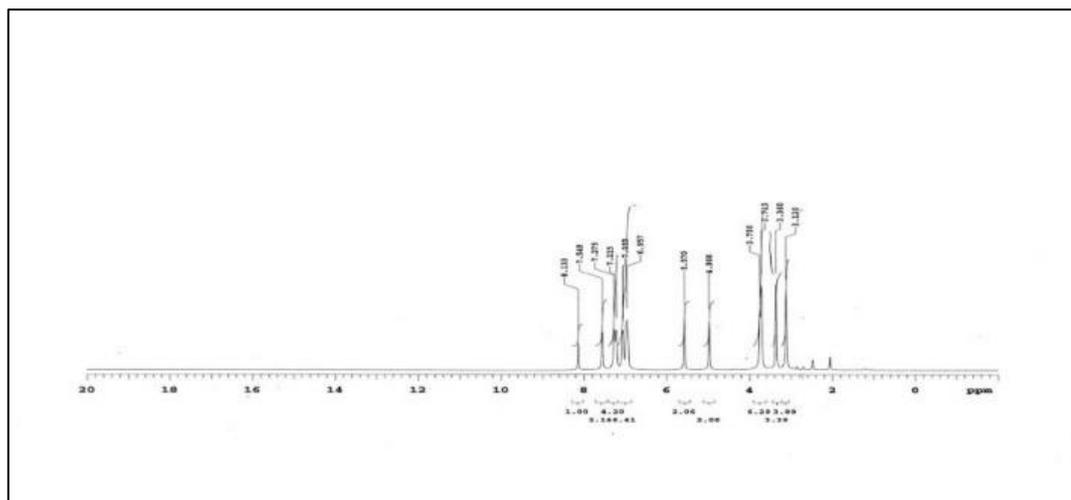
S68. ¹H NMR spectra of compound (6b)S69. ¹³C NMR (APT) spectra of compound (6b)



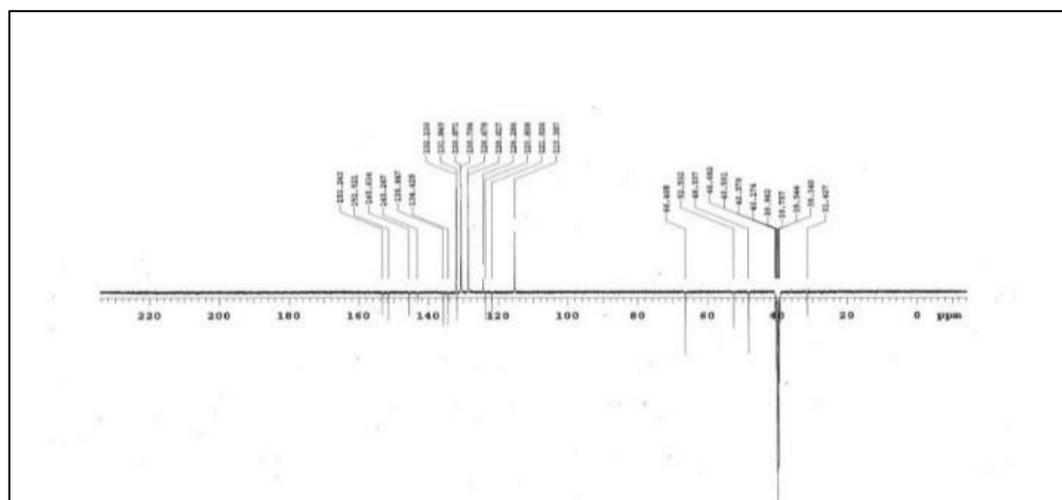
S70. Mass spectra of compound (6b)



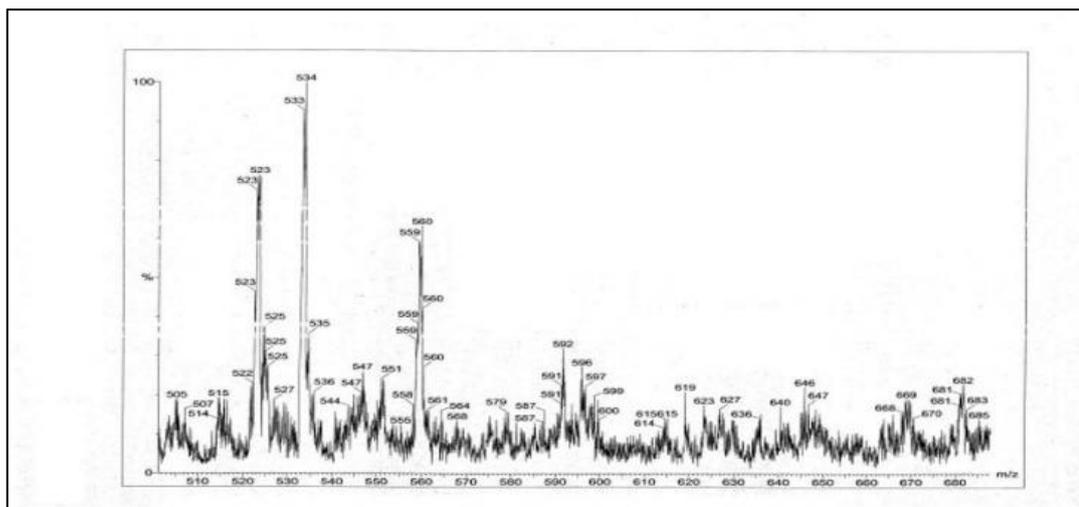
S71. FT-IR spectra of compound (6c)



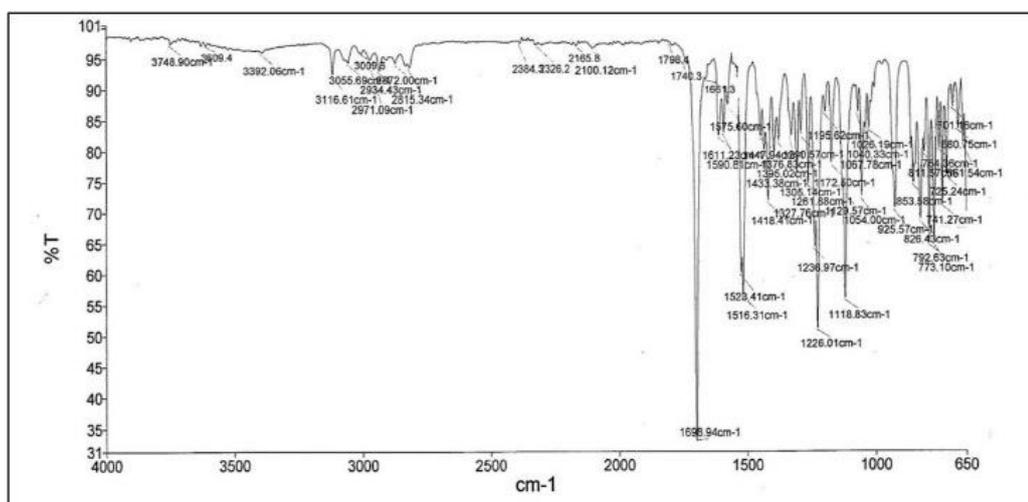
S72. ¹H NMR spectra of compound (6c)



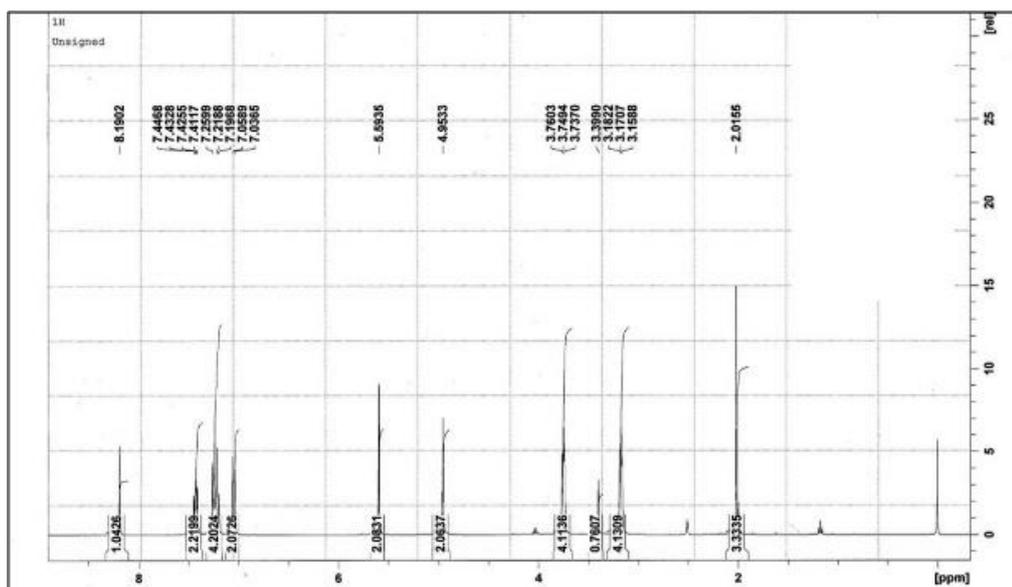
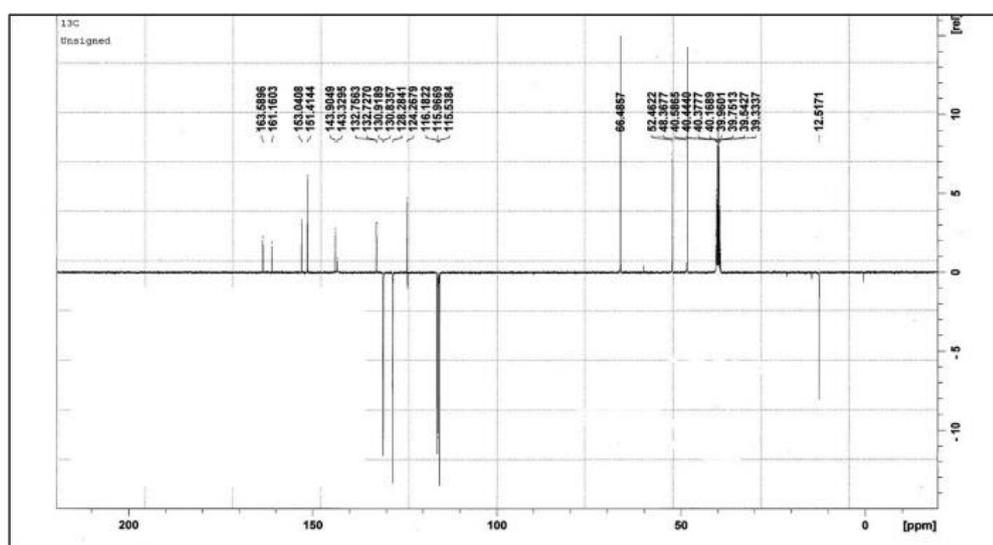
S73. ¹³C NMR (APT) spectra of compound (6c)

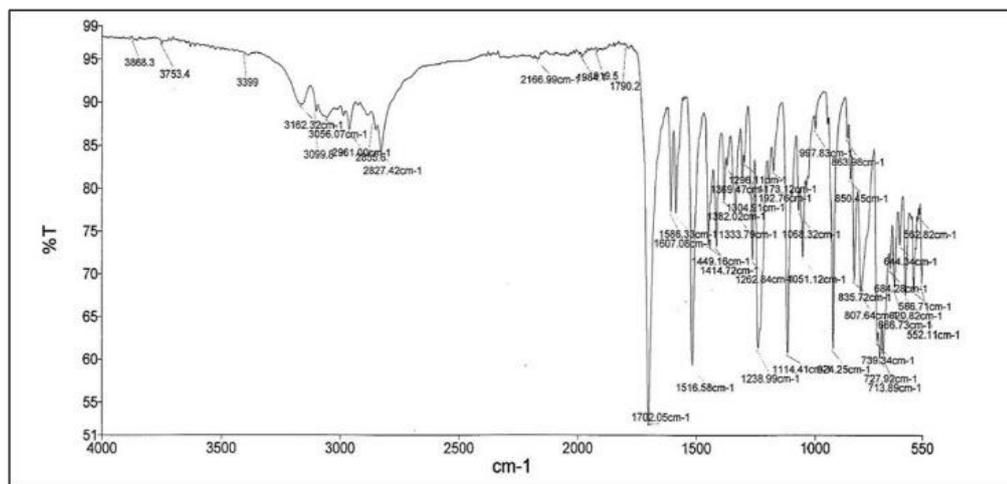


S74. Mass spectra of compound (6c)

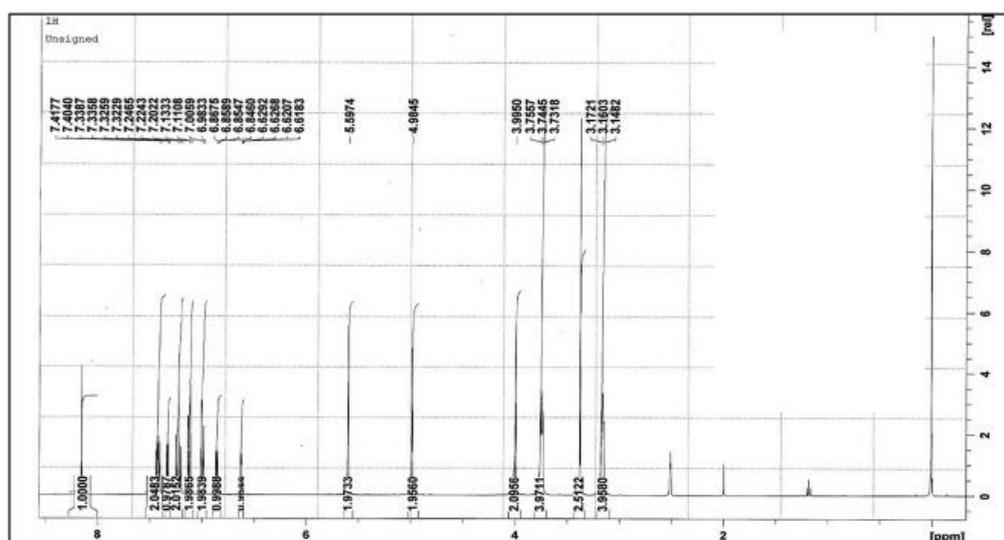


S75. FT-IR spectra of compound (7a)

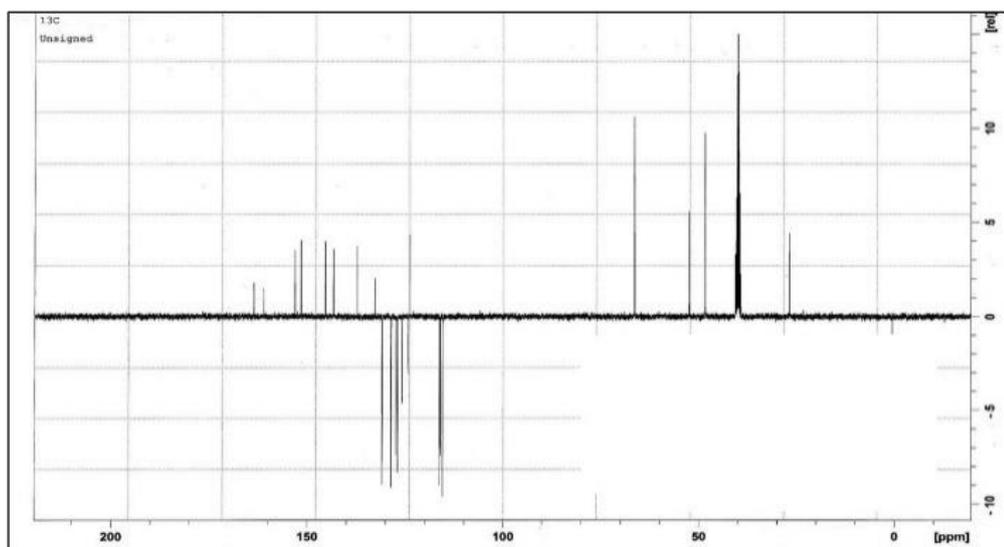
S76. ¹H NMR spectra of compound (7a)S77. ¹³C NMR (APT) spectra of compound (7a)



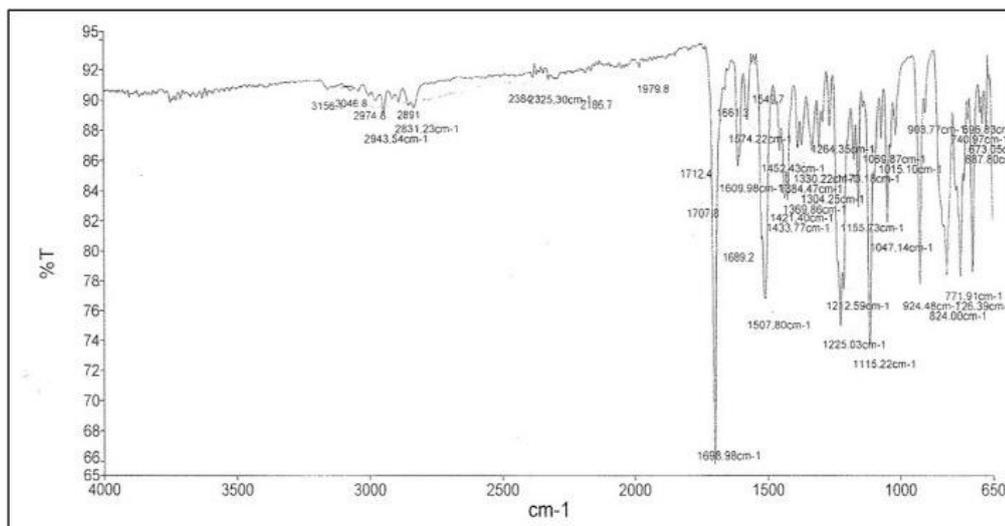
S78. FT-IR spectra of compound (7b)



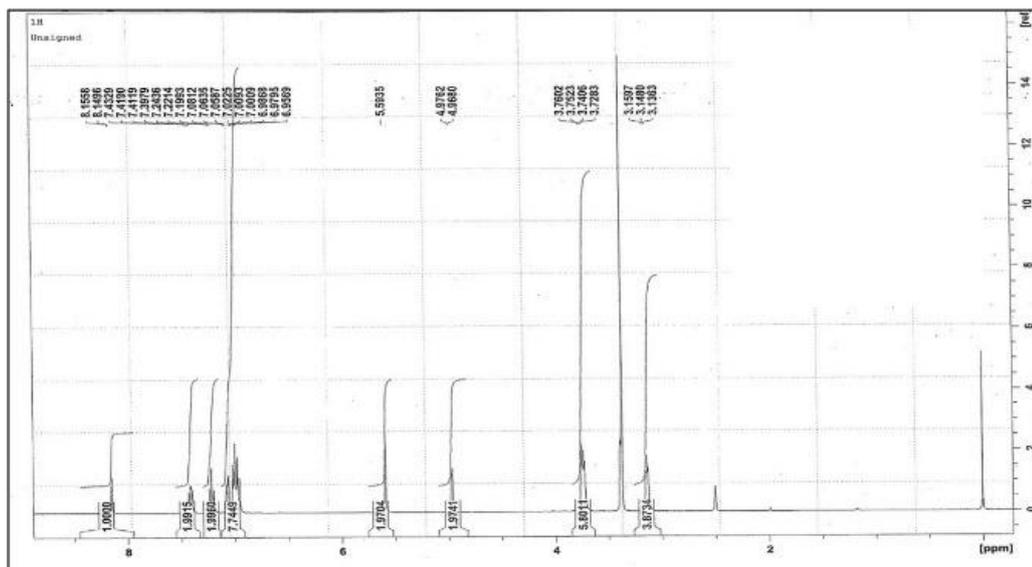
S79. ¹H NMR spectra of compound (7b)



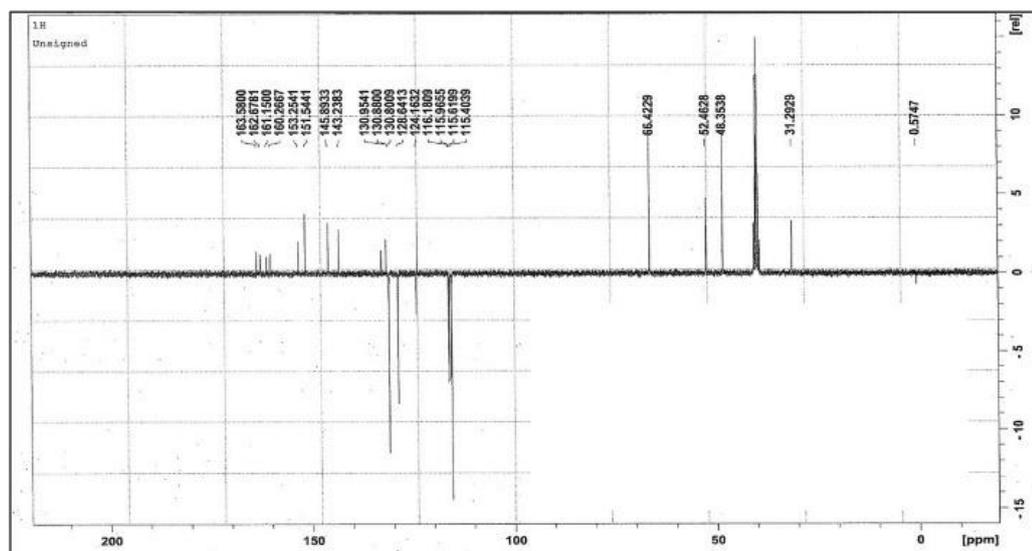
S80. ^{13}C NMR (APT) spectra of compound (7b)



S81. FT-IR spectra of compound (7c)



S82. ¹H NMR spectra of compound (7c)



S83. ¹³C NMR (APT) spectra of compound (7c)

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
31 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
22 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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S84. checkCIF/PLATON report