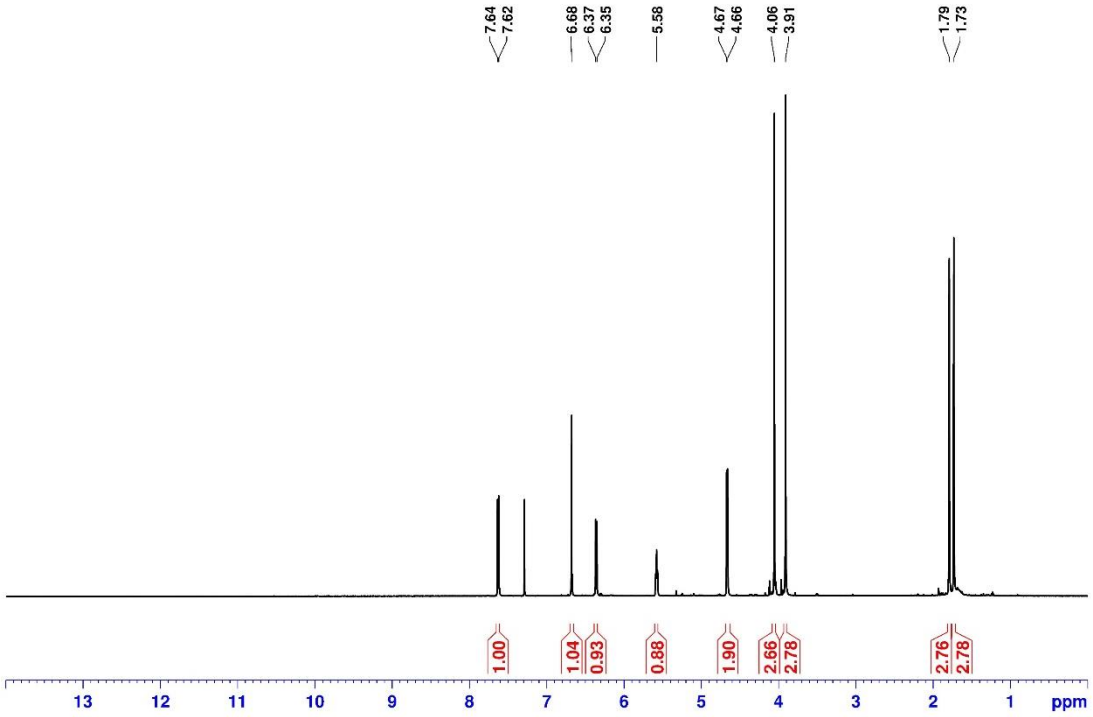
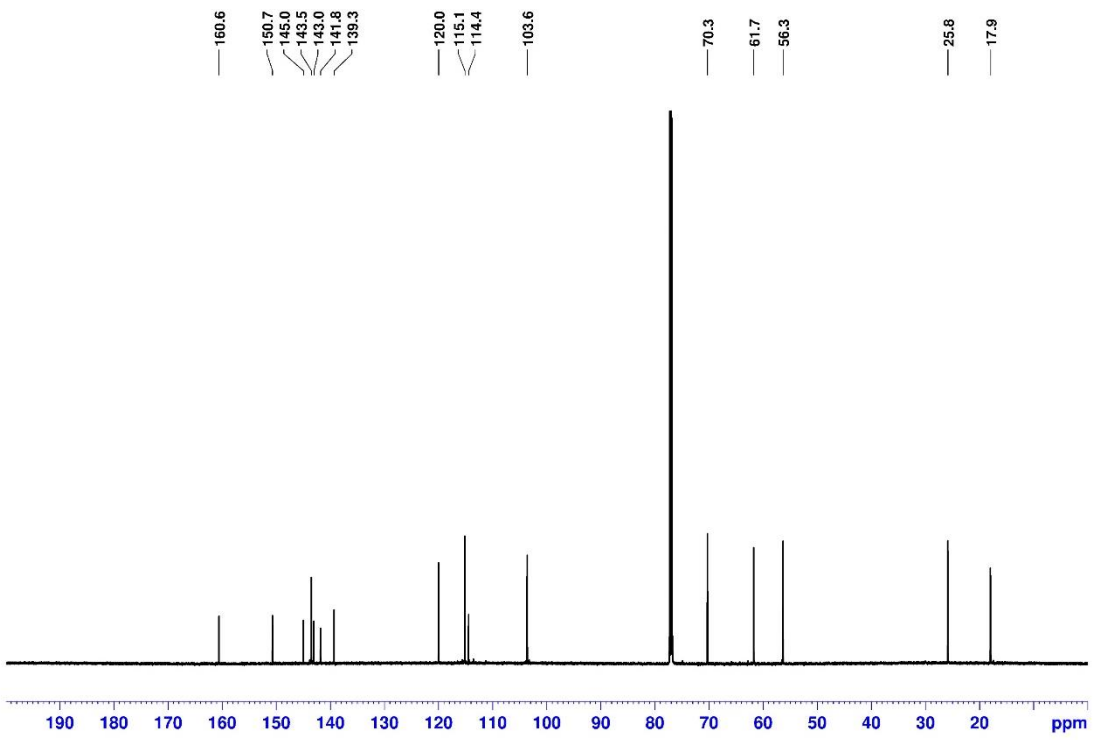
Appendix

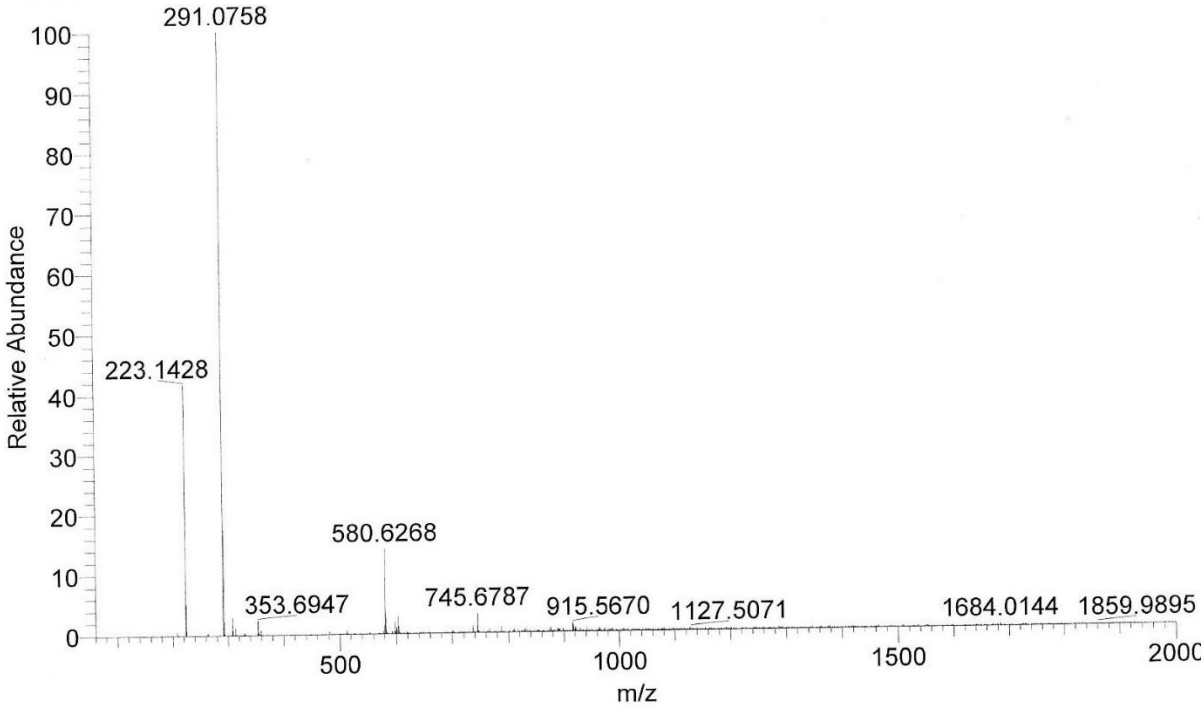
1. Spectroscopic Data of Chapter 2



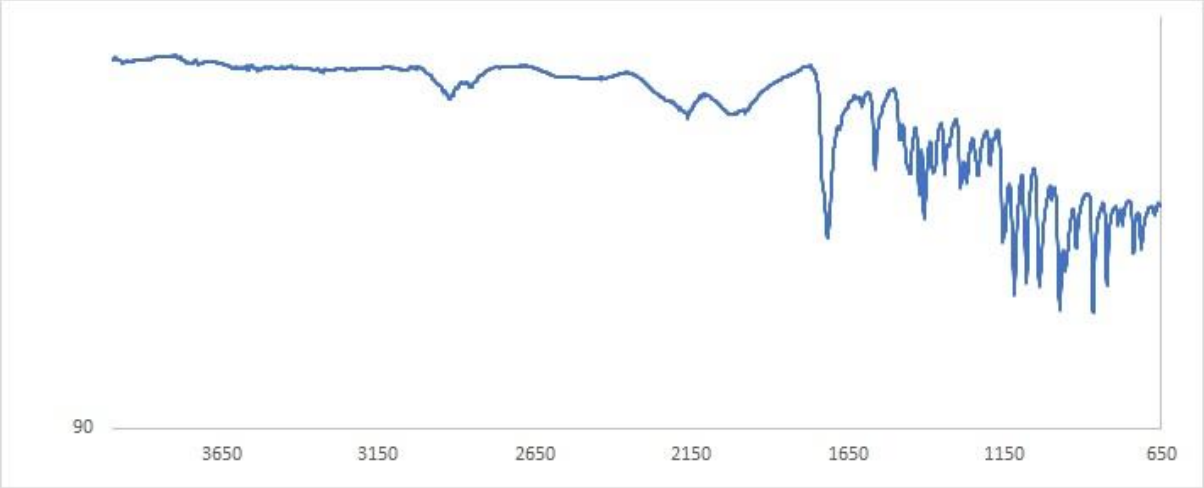
A. 1 ^{1}H NMR spectrum of **(2.01)**



A. 2 ^{13}C NMR spectrum of **(2.01)**



A. 3 ESI-HRMS of **(2.01)**, positive mode m/z 291.0758 $[M+H]^+$



A. 4 IR spectrum of **(2.01)**

A. 5 Crystal Structure Report for **(2.01)**

A specimen of $C_{16}H_{18}O_5$, approximate dimensions 0.060 mm x 0.210 mm x 0.600 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 100(2)K using an Oxford Cryosystems low temperature device using a MiTeGen micromount. See Table 1 for collection parameters and exposure time. Bruker APEX software was used to correct for Lorentz and polarization effects.

A total of 594 frames were collected. The total exposure time was 2.81 hours. The integration of the data using a monoclinic unit cell yielded a total of 10091 reflections to a maximum θ angle of 26.48° (0.80 Å resolution), of which 3113 were independent (average redundancy 3.242, completeness = 99.4%, R_{int} = 3.63%, R_{sig} = 3.97%) and 1879 (60.36%) were greater than $2\sigma(F^2)$.The final cell constants of a = 15.8263(13) Å, b = 12.4790(11) Å, c = 7.7371(6) Å, β = 97.635(3)°, volume = 1514.5(2) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I).Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.908. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6373 and 0.7454.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group $P2_1/c$, with Z = 4 for the formula unit, $C_{16}H_{18}O_5$.The final anisotropic full-matrix least-squares refinement on F^2 with 194 variables converged at R1 = 5.71%, for the observed data and wR2 = 18.17% for all data. The goodness-of-fit was 1.038. The largest peak in the final difference electron density synthesis was 0.260 $e^-/Å^3$ and the largest hole was -0.195 $e^-/Å^3$ with an RMS deviation of 0.048 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.273 g/cm^3 and F(000), 616 e^-.

Refinement Note: Crystal do not survive 100K. Data collected at RT.

For References see CIF.

Table 1: Data collection details for TCD415.

Axis	dx/mm	2θ/°	ω/°	ϕ/°	χ/°	Width/°	Frames	Time/s	Wavelength/Å	Voltage/kV	Current/mA	Temperature/K
Phi	40.000	8.00	0.00	0.00	54.76	1.00	180	1.00	0.71076	50	20.0	272
Omega	40.000	22.65	207.44	284.69	54.76	0.80	207	24.00	0.71076	50	20.0	274
Omega	40.000	22.65	207.44	49.46	54.76	0.80	207	24.00	0.71076	50	20.0	284

Table 2. Crystal data and structure refinement for TCD415.

Identification code	tcd415	
Empirical formula	$C_{16}H_{18}O_5$	
Formula weight	290.30	
Temperature	293.15 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 15.8263(13) Å	□= 90°.
	b = 12.4790(11) Å	□= 97.635(3)°.
	c = 7.7371(6) Å	□ = 90°.
Volume	1514.5(2) $Å^3$	
Z	4	
Density (calculated)	1.273 Mg/m^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	616	
Crystal size	0.6 x 0.21 x 0.06 mm^3	
Theta range for data collection	2.597 to 26.478°.	
Index ranges	-19≤h≤19, -15≤k≤15, -9≤l≤9	
Reflections collected	10091	
Independent reflections	3113 [R(int) = 0.0363]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6373	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3113 / 0 / 194	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2σ(I)]	R1 = 0.0571, wR2 = 0.1493	
R indices (all data)	R1 = 0.0967, wR2 = 0.1817	
Largest diff. peak and hole	0.260 and -0.195 $e.Å^{-3}$	

Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for TCD415. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4793(1)	5257(1)	2433(2)	54(1)
C(2)	5519(1)	4791(2)	1972(3)	55(1)
O(3)	6004(1)	5375(1)	1341(3)	72(1)
C(4)	5623(2)	3658(2)	2292(3)	58(1)
C(5)	5059(1)	3086(2)	3022(3)	53(1)
C(6)	4303(1)	3577(2)	3498(3)	47(1)
C(7)	3673(1)	3010(2)	4205(3)	53(1)
C(8)	2946(2)	3519(2)	4542(3)	55(1)
O(9)	2282(1)	3032(1)	5194(3)	73(1)
C(10)	2246(2)	1896(2)	5085(4)	74(1)
C(11)	2834(2)	4624(2)	4165(3)	57(1)
C(12)	3452(1)	5187(2)	3458(3)	54(1)
O(13)	3346(1)	6254(1)	3027(3)	71(1)
C(14)	2817(2)	6409(2)	1411(5)	94(1)
C(15)	4194(1)	4664(2)	3143(3)	48(1)
O(16)	2081(1)	5126(1)	4355(3)	72(1)
C(17)	1995(2)	5437(3)	6097(5)	96(1)
C(18)	1272(2)	6187(3)	6042(5)	91(1)
C(19)	598(2)	6085(3)	6799(4)	82(1)
C(20)	388(4)	5114(5)	7763(7)	184(3)
C(21)	-99(3)	6892(5)	6666(6)	168(2)

Table 4. Bond lengths [Å] and angles [°] for TCD415.

O(1)-C(2)	1.376(3)	C(20)-H(20C)	0.9600
O(1)-C(15)	1.374(3)	C(21)-H(21A)	0.9600
C(2)-O(3)	1.208(3)	C(21)-H(21B)	0.9600
C(2)-C(4)	1.440(3)	C(21)-H(21C)	0.9600
C(4)-H(4)	0.9300		
C(4)-C(5)	1.326(3)	C(15)-O(1)-C(2)	121.40(16)
C(5)-H(5)	0.9300	O(1)-C(2)-C(4)	116.8(2)
C(5)-C(6)	1.436(3)	O(3)-C(2)-O(1)	116.5(2)
C(6)-C(7)	1.394(3)	O(3)-C(2)-C(4)	126.7(2)
C(6)-C(15)	1.391(3)	C(2)-C(4)-H(4)	118.9
C(7)-H(7)	0.9300	C(5)-C(4)-C(2)	122.3(2)
C(7)-C(8)	1.368(3)	C(5)-C(4)-H(4)	118.9
C(8)-O(9)	1.368(3)	C(4)-C(5)-H(5)	119.7
C(8)-C(11)	1.415(3)	C(4)-C(5)-C(6)	120.63(19)
O(9)-C(10)	1.421(3)	C(6)-C(5)-H(5)	119.7
C(10)-H(10A)	0.9600	C(7)-C(6)-C(5)	123.28(18)
C(10)-H(10B)	0.9600	C(15)-C(6)-C(5)	116.9(2)
C(10)-H(10C)	0.9600	C(15)-C(6)-C(7)	119.74(19)
C(11)-C(12)	1.376(3)	C(6)-C(7)-H(7)	119.9
C(11)-O(16)	1.371(3)	C(8)-C(7)-C(6)	120.2(2)
C(12)-O(13)	1.378(3)	C(8)-C(7)-H(7)	119.9
C(12)-C(15)	1.392(3)	C(7)-C(8)-C(11)	119.9(2)
O(13)-C(14)	1.423(3)	O(9)-C(8)-C(7)	124.8(2)
C(14)-H(14A)	0.9600	O(9)-C(8)-C(11)	115.3(2)
C(14)-H(14B)	0.9600	C(8)-O(9)-C(10)	116.63(19)
C(14)-H(14C)	0.9600	O(9)-C(10)-H(10A)	109.5
O(16)-C(17)	1.426(4)	O(9)-C(10)-H(10B)	109.5
C(17)-H(17A)	0.9700	O(9)-C(10)-H(10C)	109.5
C(17)-H(17B)	0.9700	H(10A)-C(10)-H(10B)	109.5
C(17)-C(18)	1.475(4)	H(10A)-C(10)-H(10C)	109.5
C(18)-H(18)	0.9300	H(10B)-C(10)-H(10C)	109.5
C(18)-C(19)	1.289(4)	C(12)-C(11)-C(8)	120.2(2)
C(19)-C(20)	1.485(6)	O(16)-C(11)-C(8)	120.6(2)
C(19)-C(21)	1.487(5)	O(16)-C(11)-C(12)	118.9(2)
C(20)-H(20A)	0.9600	C(11)-C(12)-O(13)	121.3(2)
C(20)-H(20B)	0.9600	C(11)-C(12)-C(15)	119.38(19)

O(13)-C(12)-C(15)	119.3(2)	C(17)-C(18)-H(18)	116.2
C(12)-O(13)-C(14)	112.51(19)	C(19)-C(18)-C(17)	127.6(3)
O(13)-C(14)-H(14A)	109.5	C(19)-C(18)-H(18)	116.2
O(13)-C(14)-H(14B)	109.5	C(18)-C(19)-C(20)	124.3(4)
O(13)-C(14)-H(14C)	109.5	C(18)-C(19)-C(21)	123.6(4)
H(14A)-C(14)-H(14B)	109.5	C(20)-C(19)-C(21)	111.9(4)
H(14A)-C(14)-H(14C)	109.5	C(19)-C(20)-H(20A)	109.5
H(14B)-C(14)-H(14C)	109.5	C(19)-C(20)-H(20B)	109.5
O(1)-C(15)-C(6)	121.96(19)	C(19)-C(20)-H(20C)	109.5
O(1)-C(15)-C(12)	117.46(18)	H(20A)-C(20)-H(20B)	109.5
C(6)-C(15)-C(12)	120.6(2)	H(20A)-C(20)-H(20C)	109.5
C(11)-O(16)-C(17)	114.8(2)	H(20B)-C(20)-H(20C)	109.5
O(16)-C(17)-H(17A)	110.0	C(19)-C(21)-H(21A)	109.5
O(16)-C(17)-H(17B)	110.0	C(19)-C(21)-H(21B)	109.5
O(16)-C(17)-C(18)	108.5(3)	C(19)-C(21)-H(21C)	109.5
H(17A)-C(17)-H(17B)	108.4	H(21A)-C(21)-H(21B)	109.5
C(18)-C(17)-H(17A)	110.0	H(21A)-C(21)-H(21C)	109.5
C(18)-C(17)-H(17B)	110.0	H(21B)-C(21)-H(21C)	109.5

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for TCD415. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	55(1)	35(1)	70(1)	0(1)	-1(1)	-3(1)
C(2)	51(1)	48(1)	62(1)	-4(1)	-5(1)	-4(1)
O(3)	68(1)	57(1)	91(1)	7(1)	10(1)	-12(1)
C(4)	51(1)	46(1)	75(2)	1(1)	4(1)	6(1)
C(5)	54(1)	37(1)	65(2)	1(1)	-1(1)	6(1)
C(6)	52(1)	35(1)	52(1)	-2(1)	-3(1)	5(1)
C(7)	59(1)	38(1)	59(1)	4(1)	0(1)	4(1)
C(8)	55(1)	49(1)	61(1)	-2(1)	6(1)	0(1)
O(9)	67(1)	60(1)	95(1)	2(1)	22(1)	1(1)
C(10)	77(2)	65(2)	80(2)	2(1)	12(2)	-17(1)
C(11)	54(1)	48(1)	67(2)	-7(1)	-1(1)	9(1)
C(12)	56(1)	33(1)	70(2)	-4(1)	-6(1)	4(1)
O(13)	72(1)	35(1)	100(1)	-2(1)	-5(1)	10(1)
C(14)	93(2)	64(2)	117(3)	22(2)	-10(2)	12(2)
C(15)	50(1)	34(1)	56(1)	-5(1)	-4(1)	0(1)
O(16)	58(1)	69(1)	89(1)	-9(1)	6(1)	18(1)
C(17)	72(2)	108(2)	107(3)	-23(2)	10(2)	25(2)
C(18)	75(2)	74(2)	125(3)	-10(2)	18(2)	7(2)
C(19)	62(2)	111(2)	75(2)	-13(2)	12(2)	10(2)
C(20)	191(6)	222(7)	150(5)	50(4)	64(4)	-24(5)
C(21)	129(4)	244(6)	135(4)	-25(4)	29(3)	93(4)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for TCD415.

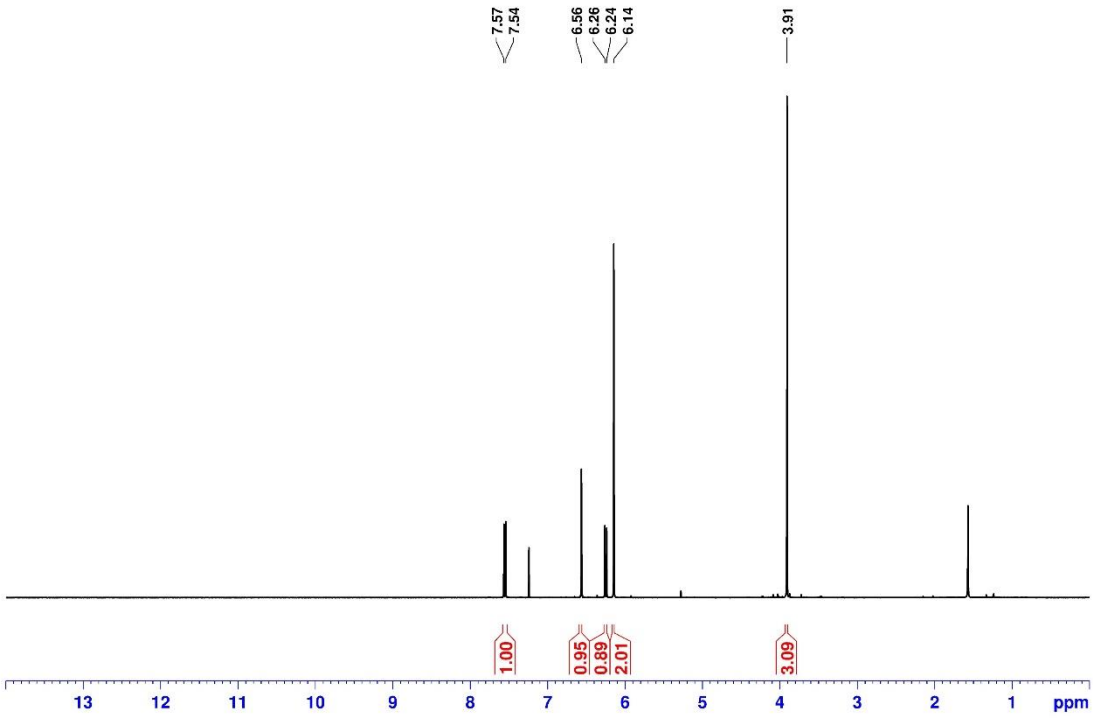
	x	y	z	U(eq)
H(4)	6102	3317	1976	69
H(5)	5155	2358	3227	64
H(7)	3745	2284	4449	64
H(10A)	2264	1678	3900	111
H(10B)	1726	1647	5461	111
H(10C)	2724	1595	5820	111
H(14A)	2987	5925	557	140
H(14B)	2874	7134	1025	140
H(14C)	2234	6274	1559	140
H(17A)	2515	5780	6632	115
H(17B)	1894	4811	6783	115
H(18)	1306	6806	5384	109
H(20A)	672	4504	7349	276
H(20B)	-217	4998	7577	276
H(20C)	572	5210	8986	276
H(21A)	107	7564	6290	252
H(21B)	-289	6980	7786	252
H(21C)	-566	6651	5837	252

Table 7. Torsion angles [°] for TCD415.

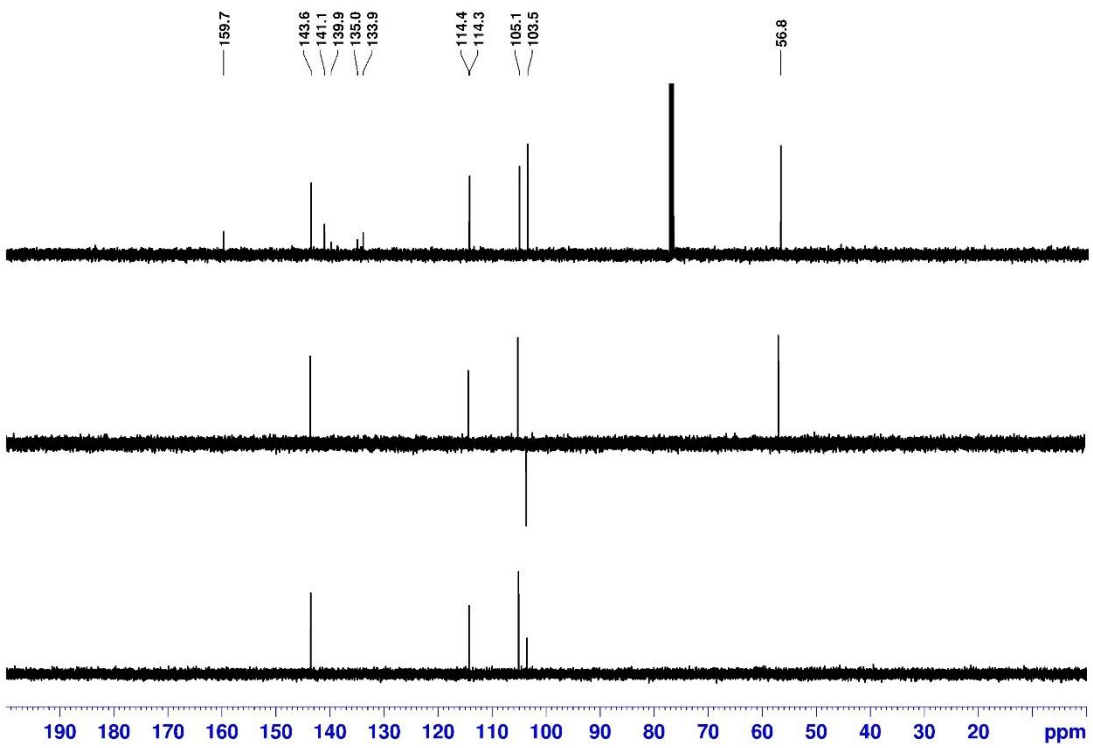
O(1)-C(2)-C(4)-C(5)	O(16)-C(17)-C(18)-C(19)
C(2)-O(1)-C(15)-C(6)	C(17)-C(18)-C(19)-C(20)
C(2)-O(1)-C(15)-C(12)	C(17)-C(18)-C(19)-C(21)
C(2)-C(4)-C(5)-C(6)	1.2(4)
O(3)-C(2)-C(4)-C(5)	178.8(2)
C(4)-C(5)-C(6)-C(7)	177.4(2)
C(4)-C(5)-C(6)-C(15)	0.5(3)
C(5)-C(6)-C(7)-C(8)	-176.5(2)
C(5)-C(6)-C(15)-O(1)	-2.4(3)
C(5)-C(6)-C(15)-C(12)	175.8(2)
C(6)-C(7)-C(8)-O(9)	178.3(2)
C(6)-C(7)-C(8)-C(11)	0.2(3)
C(7)-C(6)-C(15)-O(1)	-179.44(19)
C(7)-C(6)-C(15)-C(12)	-1.2(3)
C(7)-C(8)-O(9)-C(10)	-17.0(3)
C(7)-C(8)-C(11)-C(12)	0.1(3)
C(7)-C(8)-C(11)-O(16)	174.4(2)
C(8)-C(11)-C(12)-O(13)	177.9(2)
C(8)-C(11)-C(12)-C(15)	-1.0(3)
C(8)-C(11)-O(16)-C(17)	81.3(3)
O(9)-C(8)-C(11)-C(12)	-178.2(2)
O(9)-C(8)-C(11)-O(16)	-3.8(3)
C(11)-C(8)-O(9)-C(10)	161.2(2)
C(11)-C(12)-O(13)-C(14)	-79.3(3)
C(11)-C(12)-C(15)-O(1)	179.82(19)
C(11)-C(12)-C(15)-C(6)	1.5(3)
C(11)-O(16)-C(17)-C(18)	166.2(3)
C(12)-C(11)-O(16)-C(17)	-104.3(3)
O(13)-C(12)-C(15)-O(1)	0.9(3)
O(13)-C(12)-C(15)-C(6)	-177.33(19)
C(15)-O(1)-C(2)-O(3)	179.30(19)
C(15)-O(1)-C(2)-C(4)	-0.8(3)
C(15)-C(6)-C(7)-C(8)	0.3(3)
C(15)-C(12)-O(13)-C(14)	99.6(3)
O(16)-C(11)-C(12)-O(13)	3.4(3)
O(16)-C(11)-C(12)-C(15)	-175.4(2)

Table 8. Hydrogen bonds for TCD415 [Å and °].

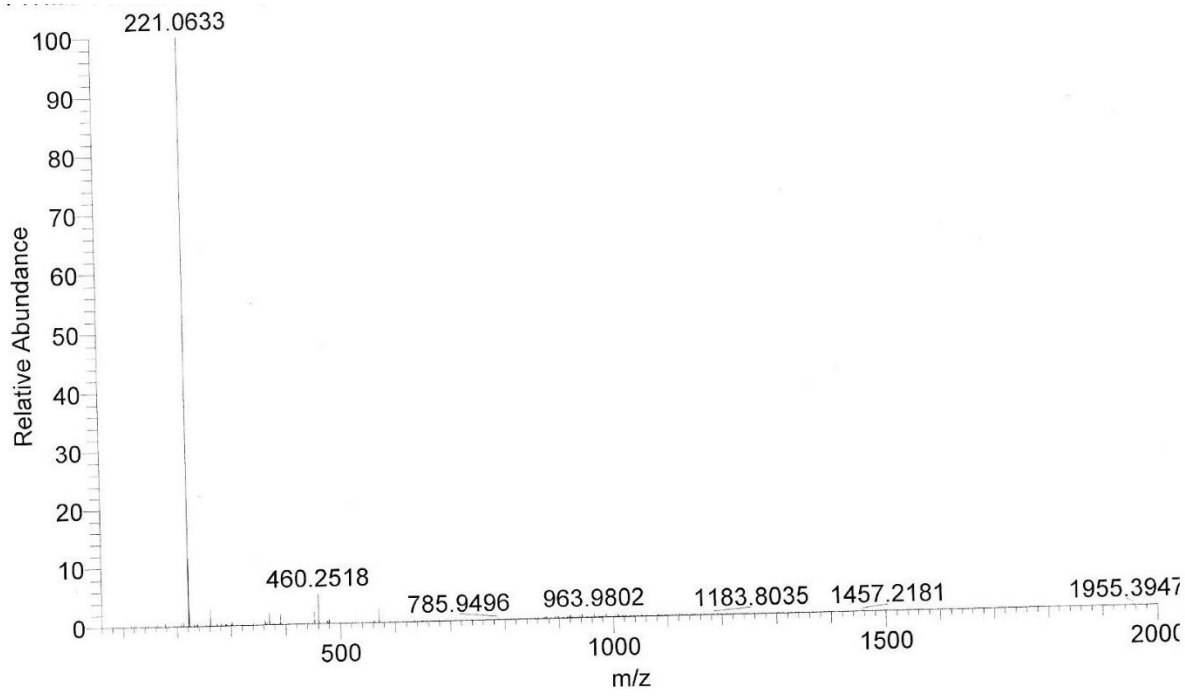
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(14)-H(14C)...O(16)	0.96	2.63	3.133(4)	113



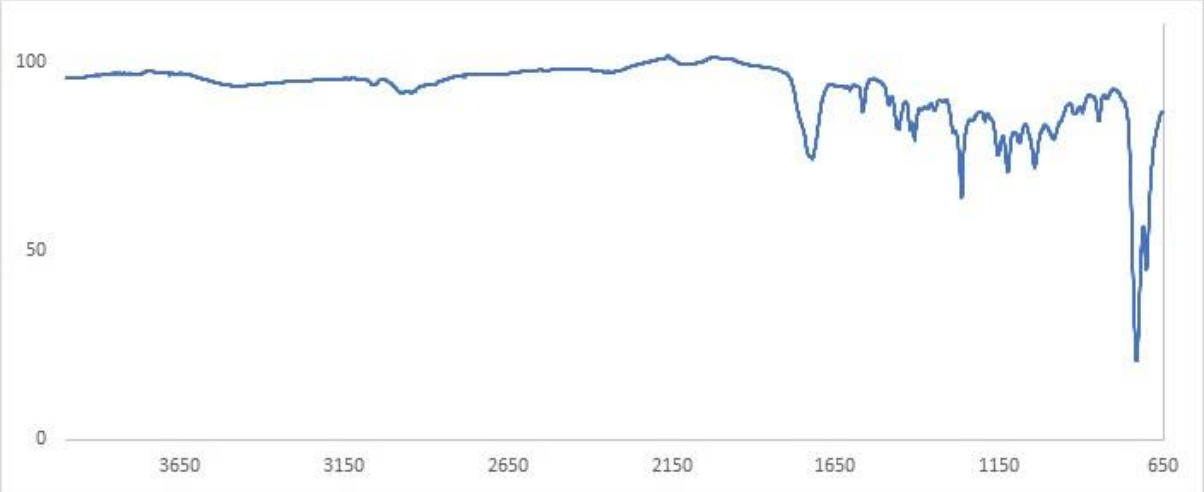
A. 6 ^{1}H NMR spectrum of **(2.02)**



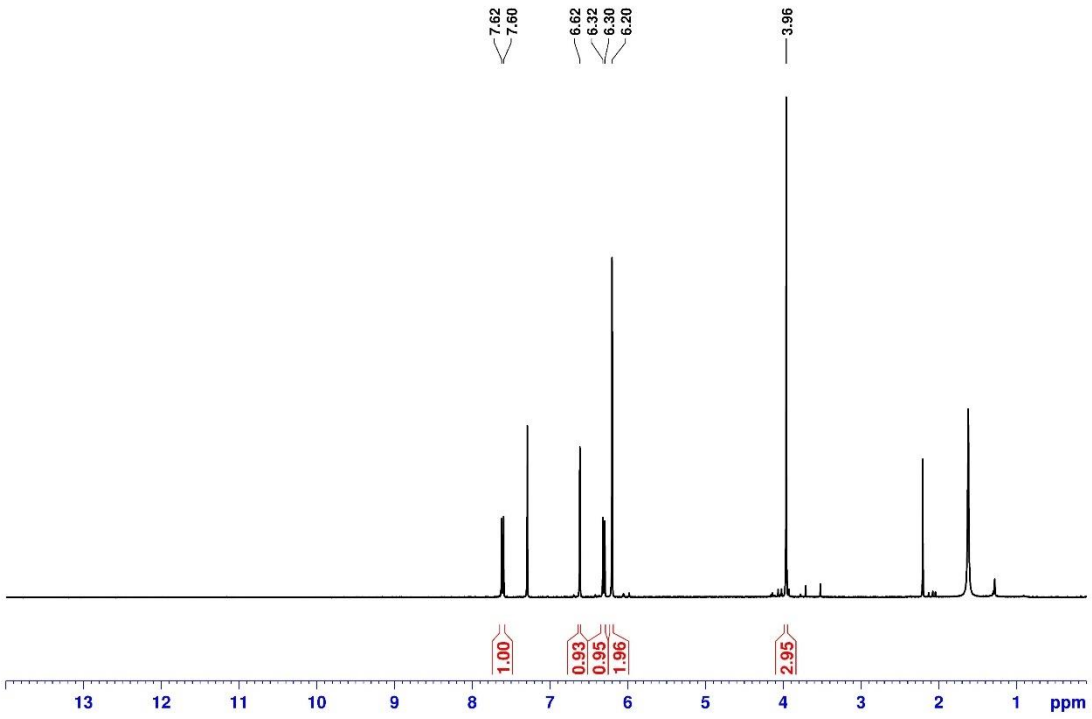
A. 7 ^{13}C NMR spectrum of **(2.02)**



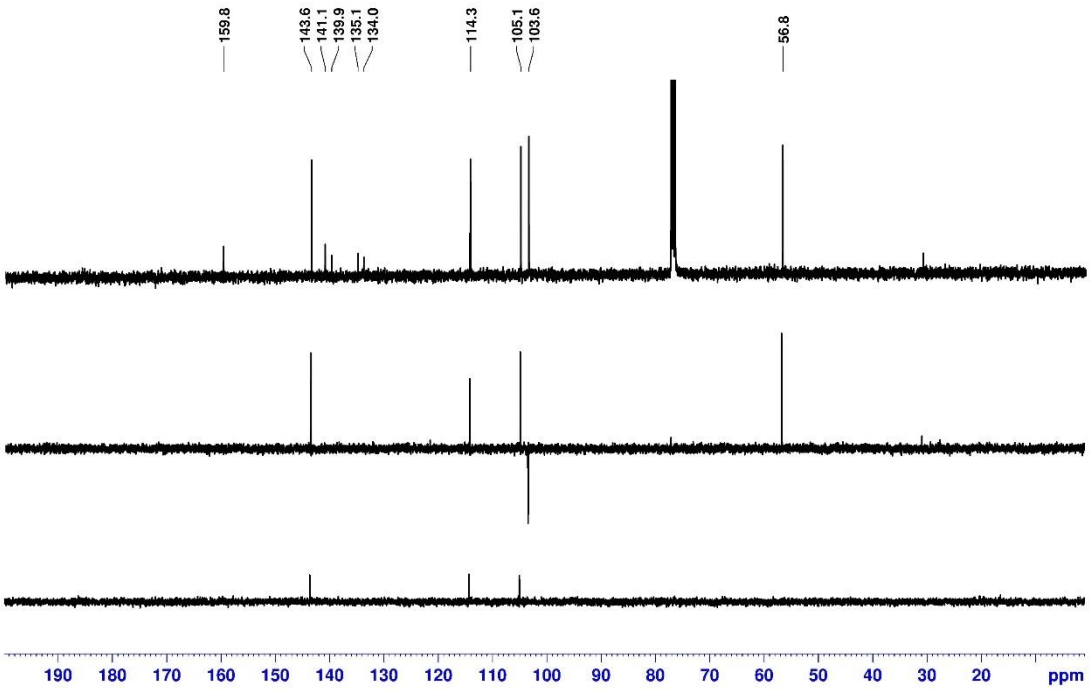
A. 8 ESI-HRMS **(2.02)**, positive mode m/z 221.0633 $[M+H]^+$



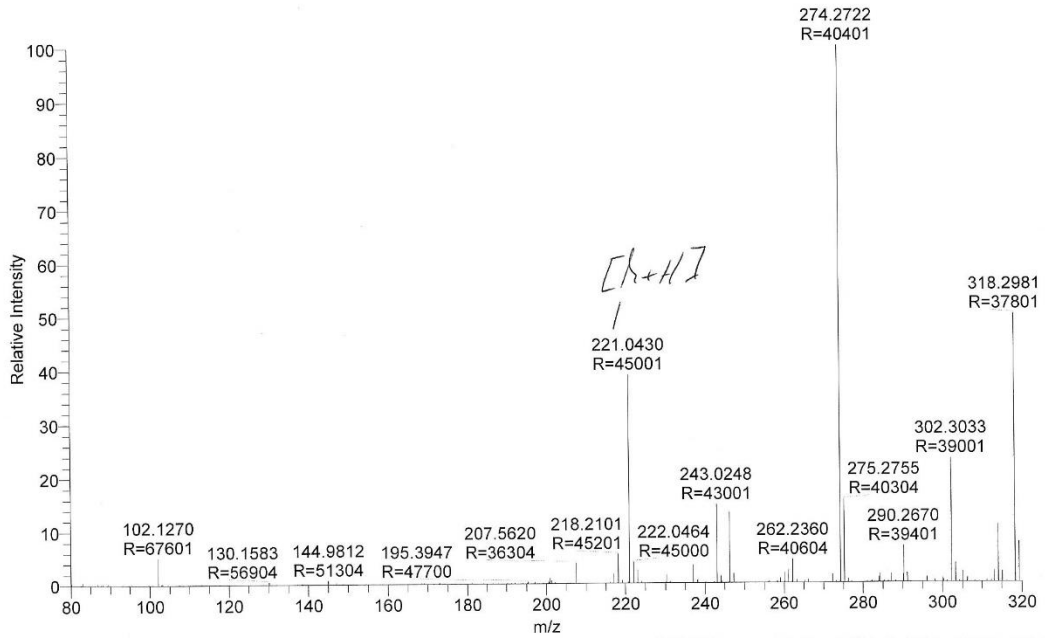
A. 9 IR spectrum **(2.02)**



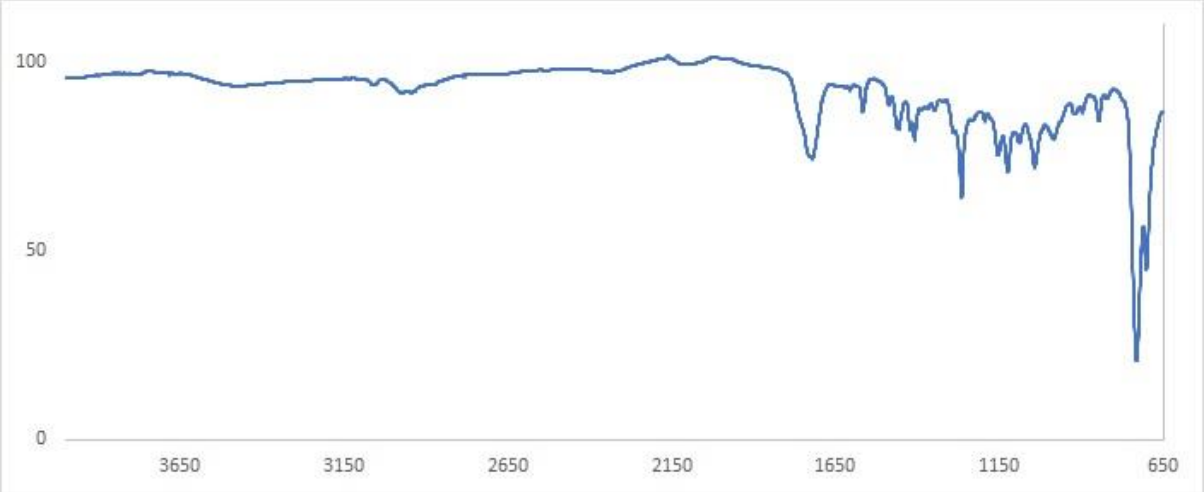
A. 10 ^{1}H NMR spectrum of **(2.03)**



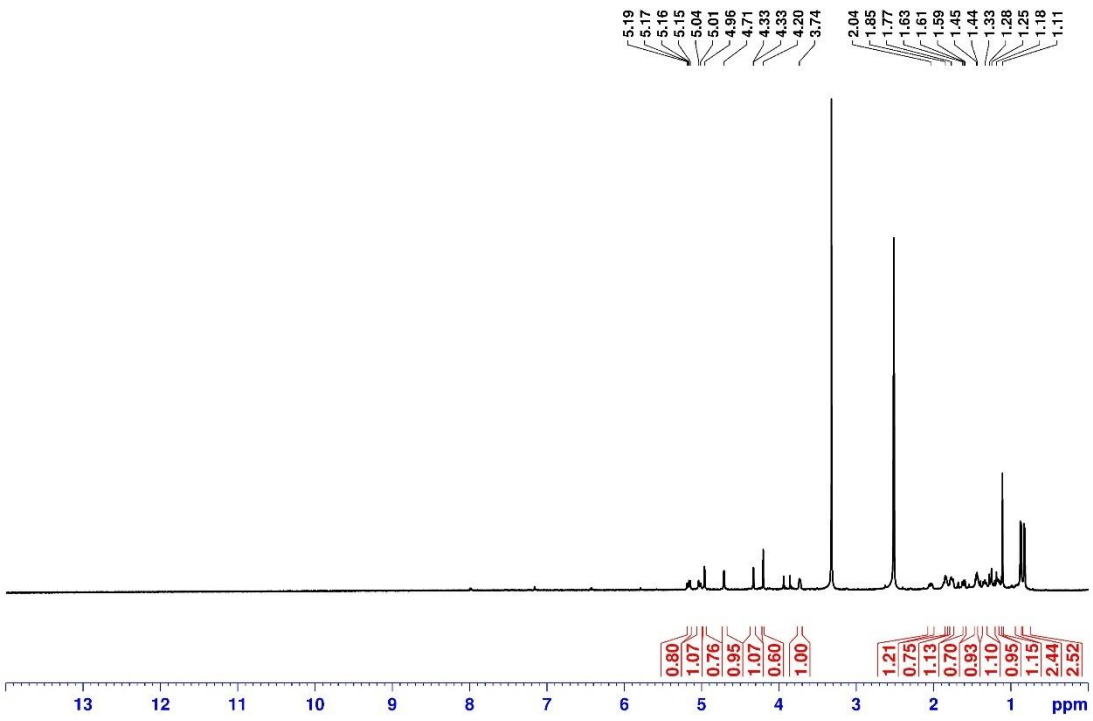
A. 11 ^{13}C NMR spectrum of **(2.03)**



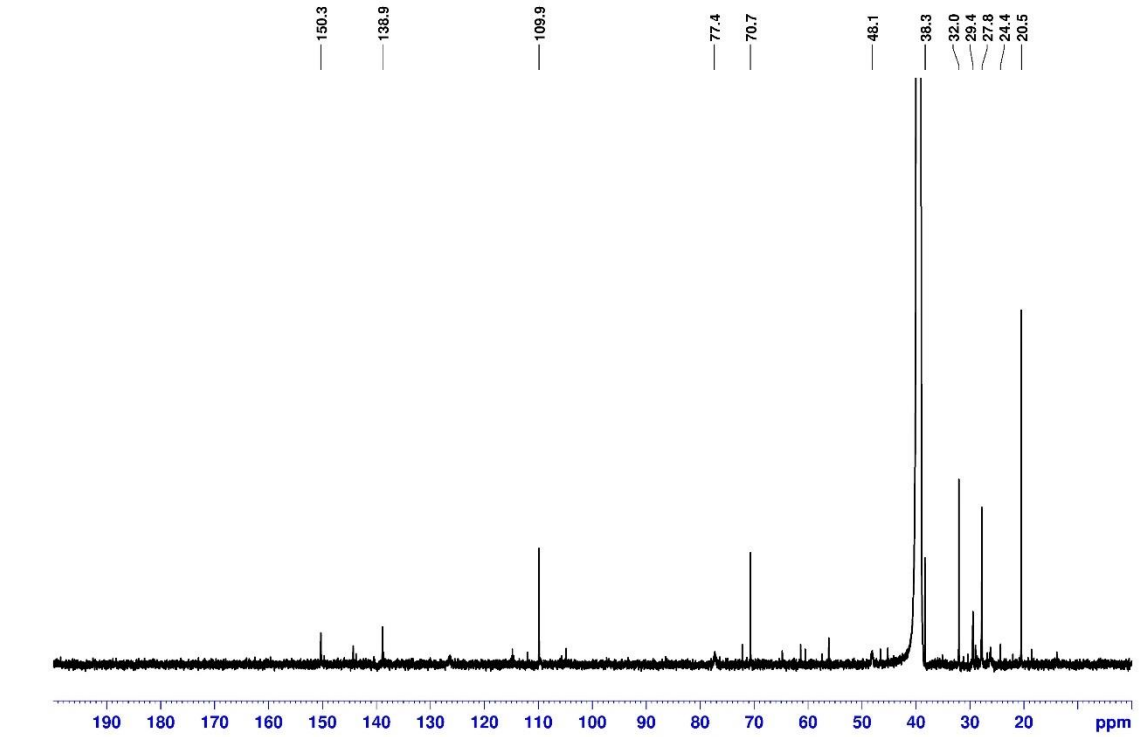
A. 12 ESI-HRMS of **(2.03)**, positive mode m/z 221.0430 $[M+H]^+$



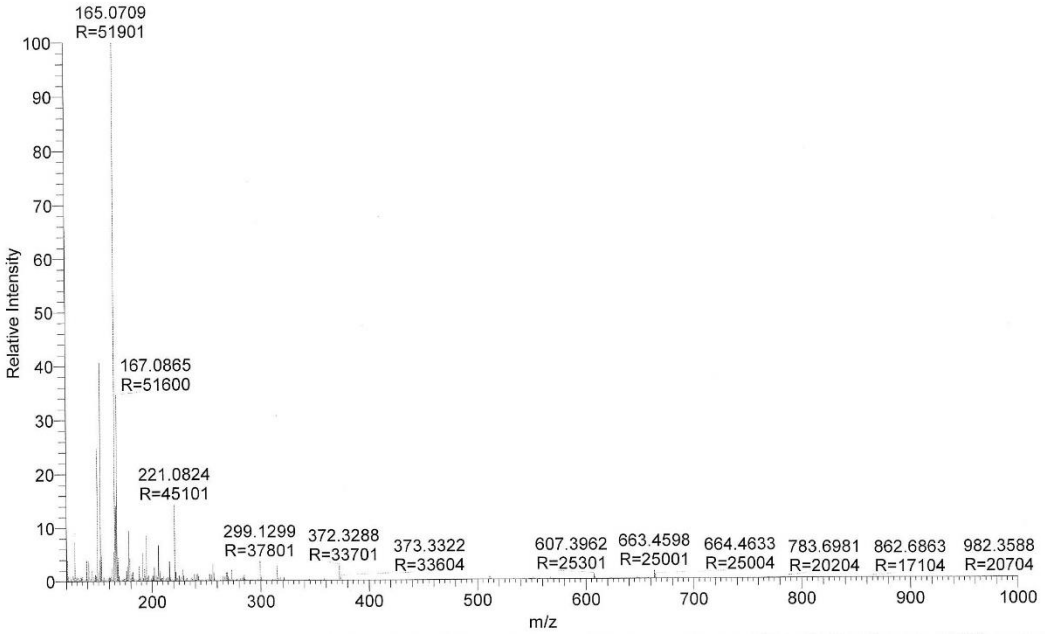
A. 13 IR spectrum of **(2.03)**



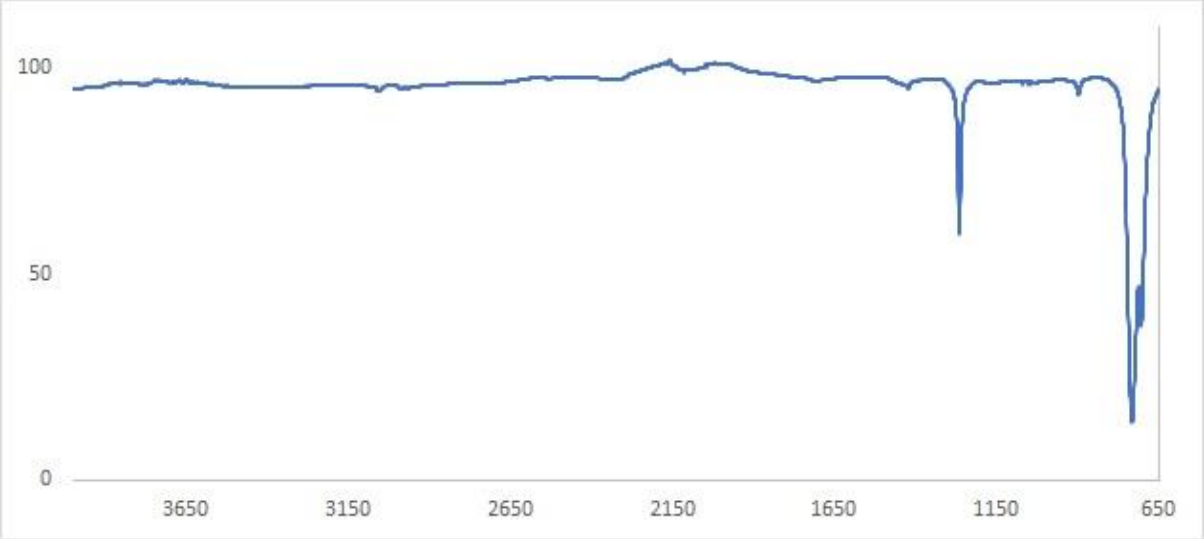
A. 14 ^{1}H NMR spectrum of **(2.04)**



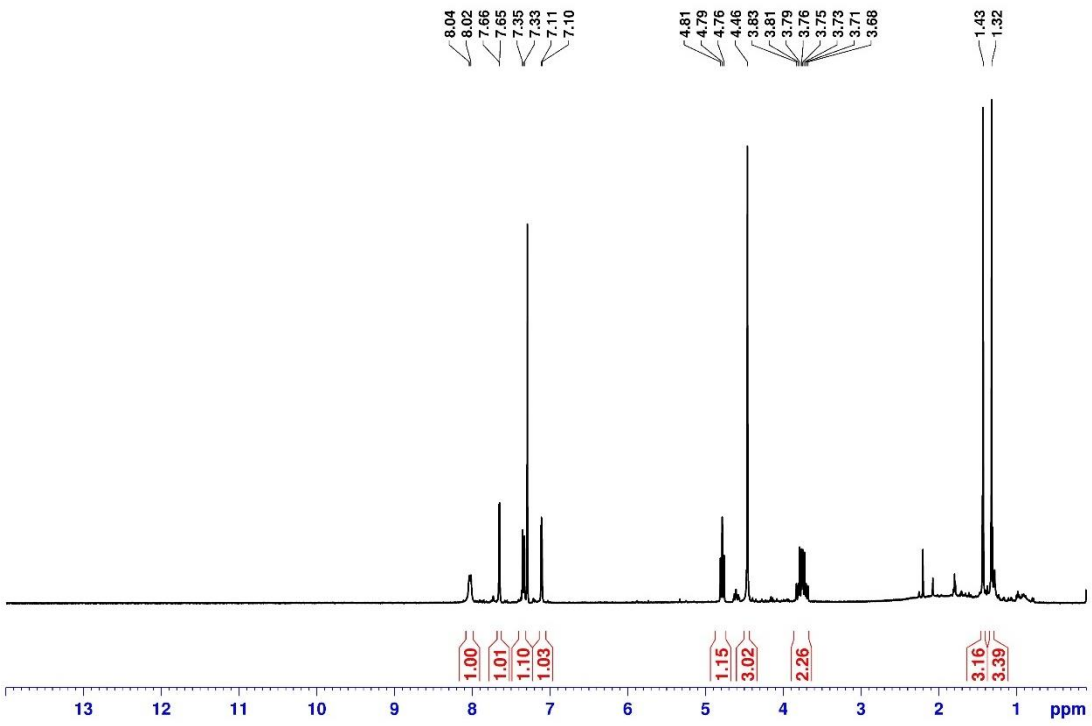
A. 15 ^{13}C NMR spectrum of **(2.04)**



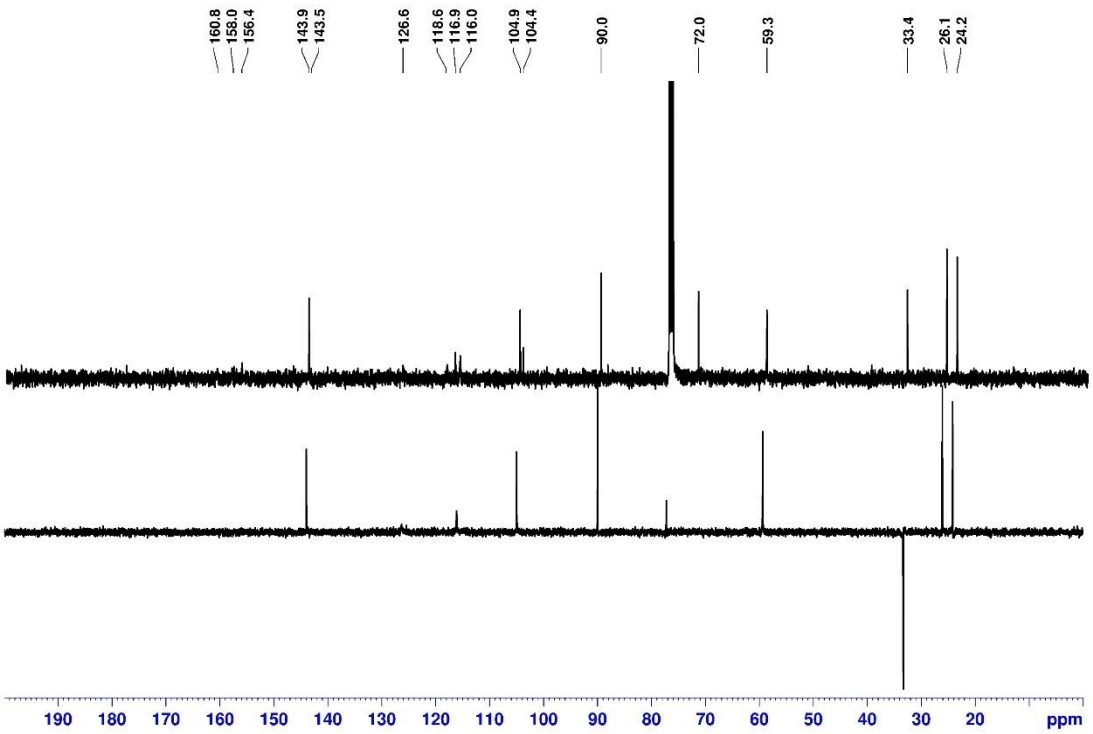
A. 16 ESI-HRMS of **(2.04)**, positive mode m/z 221.0824 $[M\text{-}H_2O+H]^+$



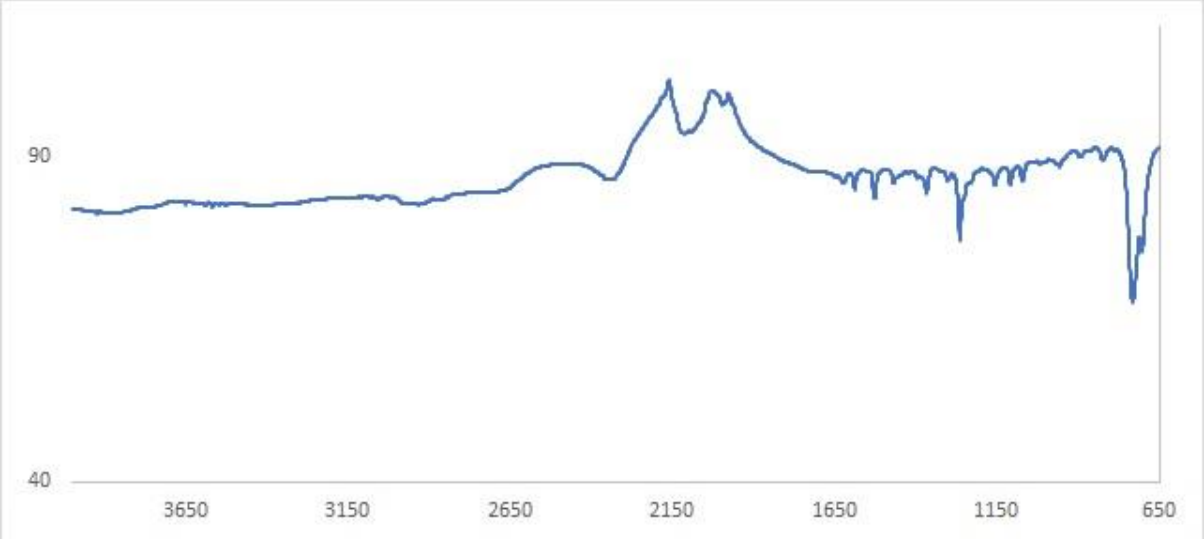
A. 17 IR spectrum of **(2.04)**



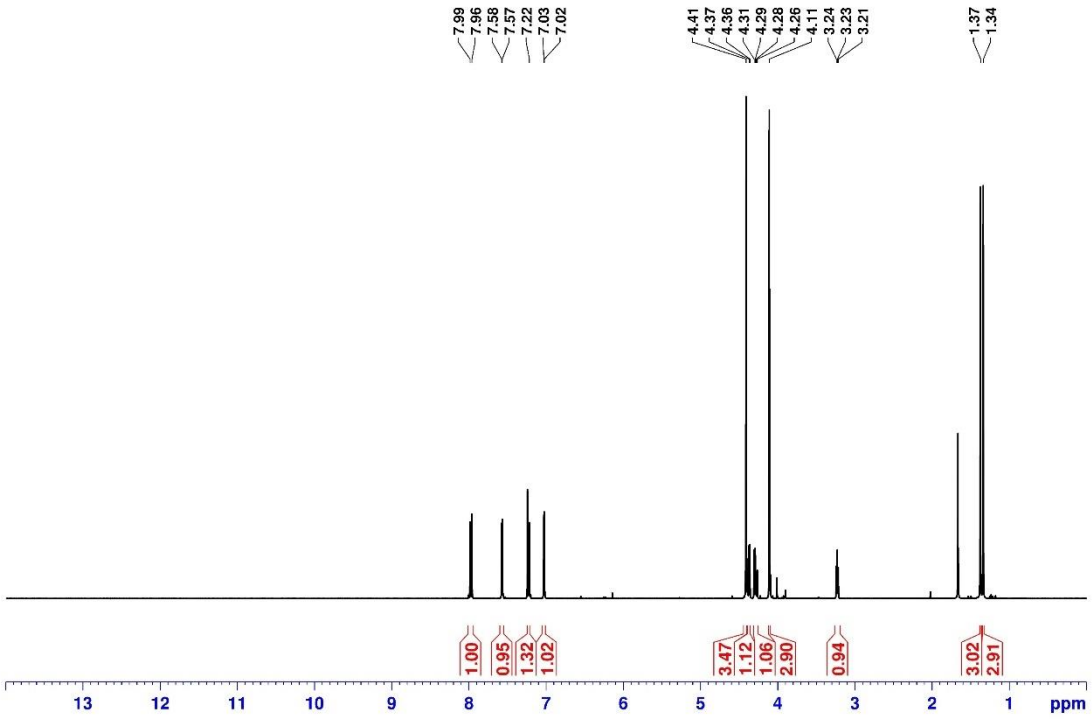
A. 18 ^{1}H NMR spectrum of **(2.05)**



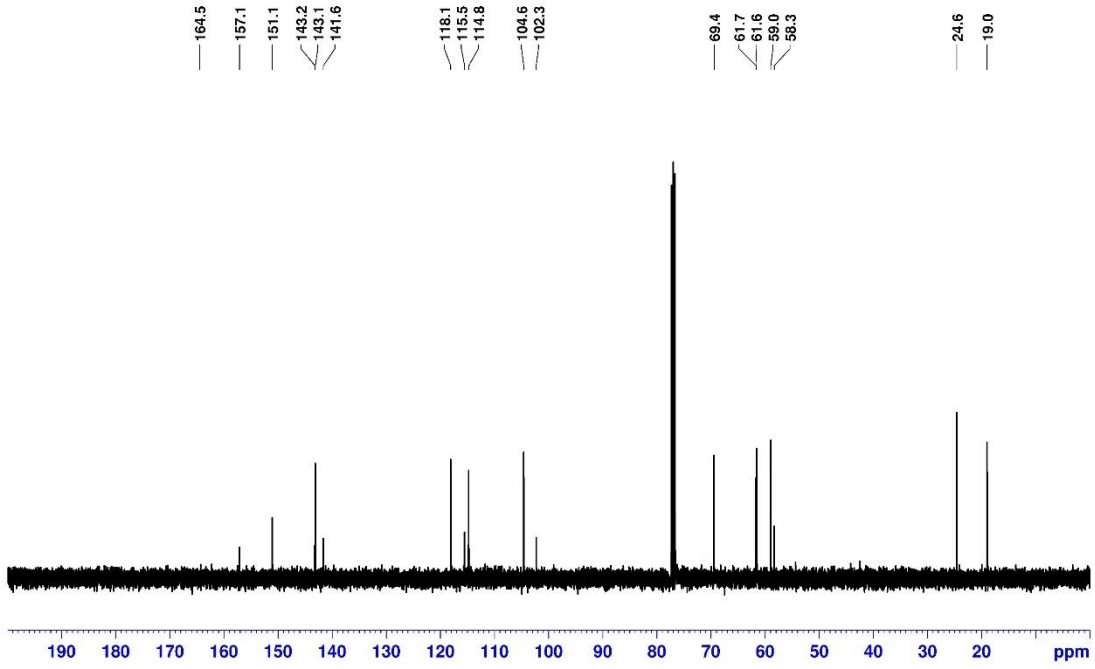
A. 19 ^{13}C NMR spectrum of **(2.05)**



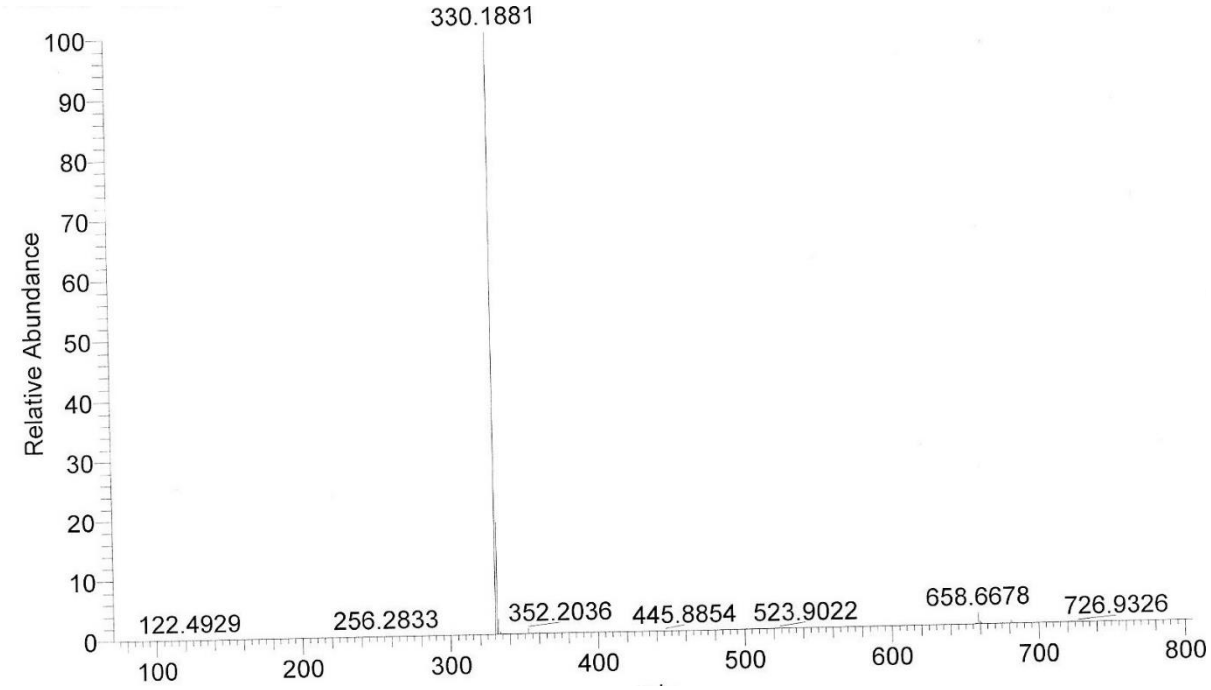
A. 20 IR spectrum of **(2.05)**



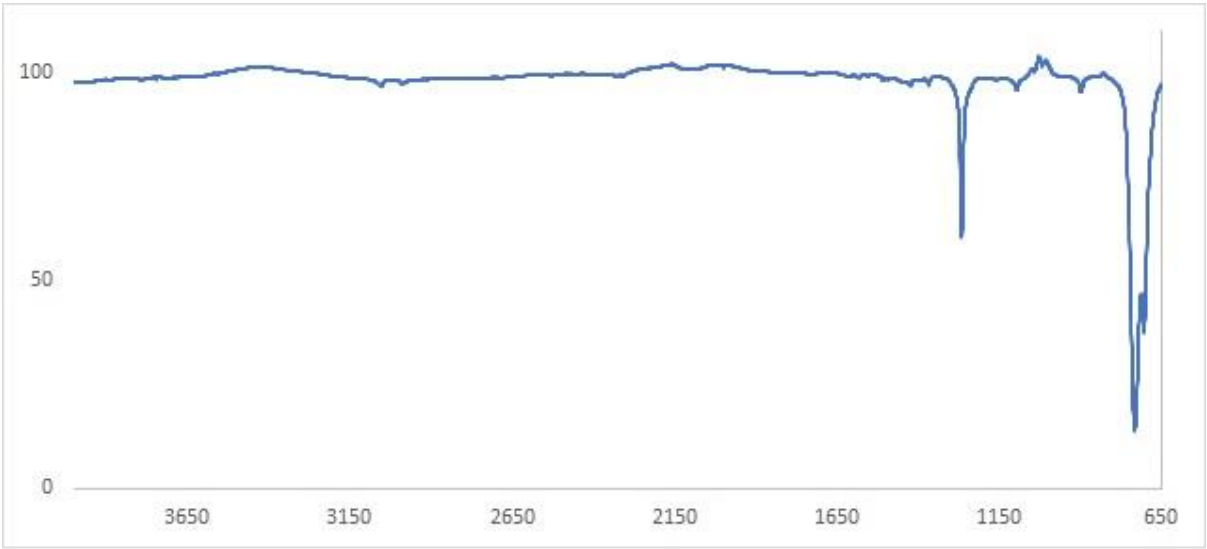
A. 21 ^{1}H NMR spectrum of **(2.06)**



A. 22 ^{13}C NMR spectrum of **(2.06)**



A. 23 ESI-MS of **(2.06)**, positive mode m/z 330.1881 $[M+H]^+$



A. 24 IR spectrum of **(2.06)**

A. 25 Crystal Structure Report for **(2.06)**

A specimen of $C_{16}H_{18}O_5$, approximate dimensions 0.060 mm x 0.210 mm x 0.600 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 100(2)K using an Oxford Cryosystems low temperature device using a MiTeGen micromount. See Table 1 for collection parameters and exposure time. Bruker APEX software was used to correct for Lorentz and polarization effects.

A total of 594 frames were collected. The total exposure time was 2.81 hours. The integration of the data using a monoclinic unit cell yielded a total of 10091 reflections to a maximum θ angle of 26.48° (0.80 Å resolution), of which 3113 were independent (average redundancy 3.242, completeness = 99.4%, R_{int} = 3.63%, R_{sig} = 3.97%) and 1879 (60.36%) were greater than $2\sigma(F^2)$.The final cell constants of a = 15.8263(13) Å, b = 12.4790(11) Å, c = 7.7371(6) Å, β = 97.635(3)°, volume = 1514.5(2) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I).Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.908. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6373 and 0.7454.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group $P2_1/c$, with Z = 4 for the formula unit, $C_{16}H_{18}O_5$.The final anisotropic full-matrix least-squares refinement on F^2 with 194 variables converged at R1 = 5.71%, for the observed data and wR2 = 18.17% for all data. The goodness-of-fit was 1.038. The largest peak in the final difference electron density synthesis was 0.260 $e^-/Å^3$ and the largest hole was -0.195 $e^-/Å^3$ with an RMS deviation of 0.048 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.273 g/cm^3 and F(000), 616 e^-.

Refinement Note: Crystal do not survive 100K. Data collected at RT.

For References see CIF.

Table 1: Data collection details for TCD415.

Axis	dx/mm	2θ/°	ω/°	φ/°	χ/°	Width/°	Frames	Time/s	Wavelength/Å	Voltage/kV	Current/mA	Temperature/K
Phi	40.000	8.00	0.00	0.00	54.76	1.00	180	1.00	0.71076	50	20.0	272
Omega	40.000	22.65	207.44	284.69	54.76	0.80	207	24.00	0.71076	50	20.0	274
Omega	40.000	22.65	207.44	49.46	54.76	0.80	207	24.00	0.71076	50	20.0	284

Table 2. Crystal data and structure refinement for TCD415.

Identification code	tcd415	
Empirical formula	$C_{16}H_{18}O_5$	
Formula weight	290.30	
Temperature	293.15 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 15.8263(13) Å	α= 90°.
	b = 12.4790(11) Å	β= 97.635(3)°.
	c = 7.7371(6) Å	γ = 90°.
Volume	1514.5(2) $Å^3$	
Z	4	
Density (calculated)	1.273 Mg/m^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	616	
Crystal size	0.6 x 0.21 x 0.06 mm^3	
Theta range for data collection	2.597 to 26.478°.	
Index ranges	-19≤h≤19, -15≤k≤15, -9≤l≤9	
Reflections collected	10091	
Independent reflections	3113 [R(int) = 0.0363]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6373	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3113 / 0 / 194	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2σ(I)]	R1 = 0.0571, wR2 = 0.1493	
R indices (all data)	R1 = 0.0967, wR2 = 0.1817	
Largest diff. peak and hole	0.260 and -0.195 $e.Å^{-3}$	

Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for TCD415. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4793(1)	5257(1)	2433(2)	54(1)
C(2)	5519(1)	4791(2)	1972(3)	55(1)
O(3)	6004(1)	5375(1)	1341(3)	72(1)
C(4)	5623(2)	3658(2)	2292(3)	58(1)
C(5)	5059(1)	3086(2)	3022(3)	53(1)
C(6)	4303(1)	3577(2)	3498(3)	47(1)
C(7)	3673(1)	3010(2)	4205(3)	53(1)
C(8)	2946(2)	3519(2)	4542(3)	55(1)
O(9)	2282(1)	3032(1)	5194(3)	73(1)
C(10)	2246(2)	1896(2)	5085(4)	74(1)
C(11)	2834(2)	4624(2)	4165(3)	57(1)
C(12)	3452(1)	5187(2)	3458(3)	54(1)
O(13)	3346(1)	6254(1)	3027(3)	71(1)
C(14)	2817(2)	6409(2)	1411(5)	94(1)
C(15)	4194(1)	4664(2)	3143(3)	48(1)
O(16)	2081(1)	5126(1)	4355(3)	72(1)
C(17)	1995(2)	5437(3)	6097(5)	96(1)
C(18)	1272(2)	6187(3)	6042(5)	91(1)
C(19)	598(2)	6085(3)	6799(4)	82(1)
C(20)	388(4)	5114(5)	7763(7)	184(3)
C(21)	-99(3)	6892(5)	6666(6)	168(2)

Table 4. Bond lengths [Å] and angles [°] for TCD415.

O(1)-C(2)	1.376(3)	C(20)-H(20C)	0.9600
O(1)-C(15)	1.374(3)	C(21)-H(21A)	0.9600
C(2)-O(3)	1.208(3)	C(21)-H(21B)	0.9600
C(2)-C(4)	1.440(3)	C(21)-H(21C)	0.9600
C(4)-H(4)	0.9300		
C(4)-C(5)	1.326(3)	C(15)-O(1)-C(2)	121.40(16)
C(5)-H(5)	0.9300	O(1)-C(2)-C(4)	116.8(2)
C(5)-C(6)	1.436(3)	O(3)-C(2)-O(1)	116.5(2)
C(6)-C(7)	1.394(3)	O(3)-C(2)-C(4)	126.7(2)
C(6)-C(15)	1.391(3)	C(2)-C(4)-H(4)	118.9
C(7)-H(7)	0.9300	C(5)-C(4)-C(2)	122.3(2)
C(7)-C(8)	1.368(3)	C(5)-C(4)-H(4)	118.9
C(8)-O(9)	1.368(3)	C(4)-C(5)-H(5)	119.7
C(8)-C(11)	1.415(3)	C(4)-C(5)-C(6)	120.63(19)
O(9)-C(10)	1.421(3)	C(6)-C(5)-H(5)	119.7
C(10)-H(10A)	0.9600	C(7)-C(6)-C(5)	123.28(18)
C(10)-H(10B)	0.9600	C(15)-C(6)-C(5)	116.9(2)
C(10)-H(10C)	0.9600	C(15)-C(6)-C(7)	119.74(19)
C(11)-C(12)	1.376(3)	C(6)-C(7)-H(7)	119.9
C(11)-O(16)	1.371(3)	C(8)-C(7)-C(6)	120.2(2)
C(12)-O(13)	1.378(3)	C(8)-C(7)-H(7)	119.9
C(12)-C(15)	1.392(3)	C(7)-C(8)-C(11)	119.9(2)
O(13)-C(14)	1.423(3)	O(9)-C(8)-C(7)	124.8(2)
C(14)-H(14A)	0.9600	O(9)-C(8)-C(11)	115.3(2)
C(14)-H(14B)	0.9600	C(8)-O(9)-C(10)	116.63(19)
C(14)-H(14C)	0.9600	O(9)-C(10)-H(10A)	109.5
O(16)-C(17)	1.426(4)	O(9)-C(10)-H(10B)	109.5
C(17)-H(17A)	0.9700	O(9)-C(10)-H(10C)	109.5
C(17)-H(17B)	0.9700	H(10A)-C(10)-H(10B)	109.5
C(17)-C(18)	1.475(4)	H(10A)-C(10)-H(10C)	109.5
C(18)-H(18)	0.9300	H(10B)-C(10)-H(10C)	109.5
C(18)-C(19)	1.289(4)	C(12)-C(11)-C(8)	120.2(2)
C(19)-C(20)	1.485(6)	O(16)-C(11)-C(8)	120.6(2)
C(19)-C(21)	1.487(5)	O(16)-C(11)-C(12)	118.9(2)
C(20)-H(20A)	0.9600	C(11)-C(12)-O(13)	121.3(2)
C(20)-H(20B)	0.9600	C(11)-C(12)-C(15)	119.38(19)

O(13)-C(12)-C(15)	119.3(2)	C(17)-C(18)-H(18)	116.2
C(12)-O(13)-C(14)	112.51(19)	C(19)-C(18)-C(17)	127.6(3)
O(13)-C(14)-H(14A)	109.5	C(19)-C(18)-H(18)	116.2
O(13)-C(14)-H(14B)	109.5	C(18)-C(19)-C(20)	124.3(4)
O(13)-C(14)-H(14C)	109.5	C(18)-C(19)-C(21)	123.6(4)
H(14A)-C(14)-H(14B)	109.5	C(20)-C(19)-C(21)	111.9(4)
H(14A)-C(14)-H(14C)	109.5	C(19)-C(20)-H(20A)	109.5
H(14B)-C(14)-H(14C)	109.5	C(19)-C(20)-H(20B)	109.5
O(1)-C(15)-C(6)	121.96(19)	C(19)-C(20)-H(20C)	109.5
O(1)-C(15)-C(12)	117.46(18)	H(20A)-C(20)-H(20B)	109.5
C(6)-C(15)-C(12)	120.6(2)	H(20A)-C(20)-H(20C)	109.5
C(11)-O(16)-C(17)	114.8(2)	H(20B)-C(20)-H(20C)	109.5
O(16)-C(17)-H(17A)	110.0	C(19)-C(21)-H(21A)	109.5
O(16)-C(17)-H(17B)	110.0	C(19)-C(21)-H(21B)	109.5
O(16)-C(17)-C(18)	108.5(3)	C(19)-C(21)-H(21C)	109.5
H(17A)-C(17)-H(17B)	108.4	H(21A)-C(21)-H(21B)	109.5
C(18)-C(17)-H(17A)	110.0	H(21A)-C(21)-H(21C)	109.5
C(18)-C(17)-H(17B)	110.0	H(21B)-C(21)-H(21C)	109.5

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for TCD415. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	55(1)	35(1)	70(1)	0(1)	-1(1)	-3(1)
C(2)	51(1)	48(1)	62(1)	-4(1)	-5(1)	-4(1)
O(3)	68(1)	57(1)	91(1)	7(1)	10(1)	-12(1)
C(4)	51(1)	46(1)	75(2)	1(1)	4(1)	6(1)
C(5)	54(1)	37(1)	65(2)	1(1)	-1(1)	6(1)
C(6)	52(1)	35(1)	52(1)	-2(1)	-3(1)	5(1)
C(7)	59(1)	38(1)	59(1)	4(1)	0(1)	4(1)
C(8)	55(1)	49(1)	61(1)	-2(1)	6(1)	0(1)
O(9)	67(1)	60(1)	95(1)	2(1)	22(1)	1(1)
C(10)	77(2)	65(2)	80(2)	2(1)	12(2)	-17(1)
C(11)	54(1)	48(1)	67(2)	-7(1)	-1(1)	9(1)
C(12)	56(1)	33(1)	70(2)	-4(1)	-6(1)	4(1)
O(13)	72(1)	35(1)	100(1)	-2(1)	-5(1)	10(1)
C(14)	93(2)	64(2)	117(3)	22(2)	-10(2)	12(2)
C(15)	50(1)	34(1)	56(1)	-5(1)	-4(1)	0(1)
O(16)	58(1)	69(1)	89(1)	-9(1)	6(1)	18(1)
C(17)	72(2)	108(2)	107(3)	-23(2)	10(2)	25(2)
C(18)	75(2)	74(2)	125(3)	-10(2)	18(2)	7(2)
C(19)	62(2)	111(2)	75(2)	-13(2)	12(2)	10(2)
C(20)	191(6)	222(7)	150(5)	50(4)	64(4)	-24(5)
C(21)	129(4)	244(6)	135(4)	-25(4)	29(3)	93(4)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for TCD415.

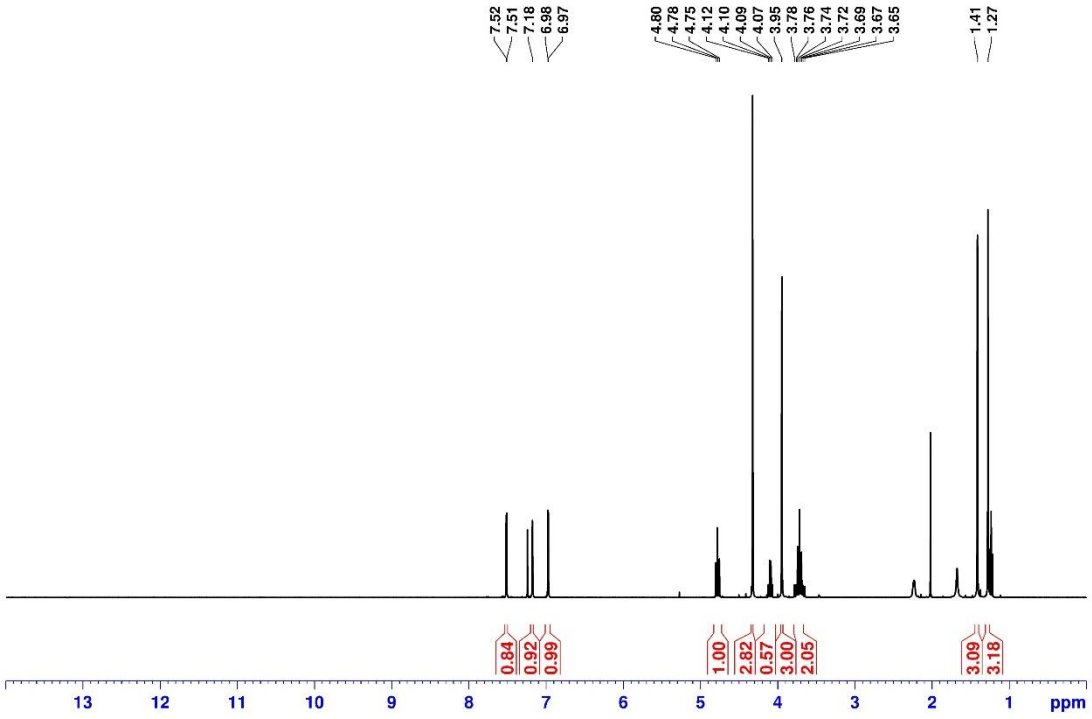
	x	y	z	U(eq)
H(4)	6102	3317	1976	69
H(5)	5155	2358	3227	64
H(7)	3745	2284	4449	64
H(10A)	2264	1678	3900	111
H(10B)	1726	1647	5461	111
H(10C)	2724	1595	5820	111
H(14A)	2987	5925	557	140
H(14B)	2874	7134	1025	140
H(14C)	2234	6274	1559	140
H(17A)	2515	5780	6632	115
H(17B)	1894	4811	6783	115
H(18)	1306	6806	5384	109
H(20A)	672	4504	7349	276
H(20B)	-217	4998	7577	276
H(20C)	572	5210	8986	276
H(21A)	107	7564	6290	252
H(21B)	-289	6980	7786	252
H(21C)	-566	6651	5837	252

Table 7. Torsion angles [°] for TCD415.

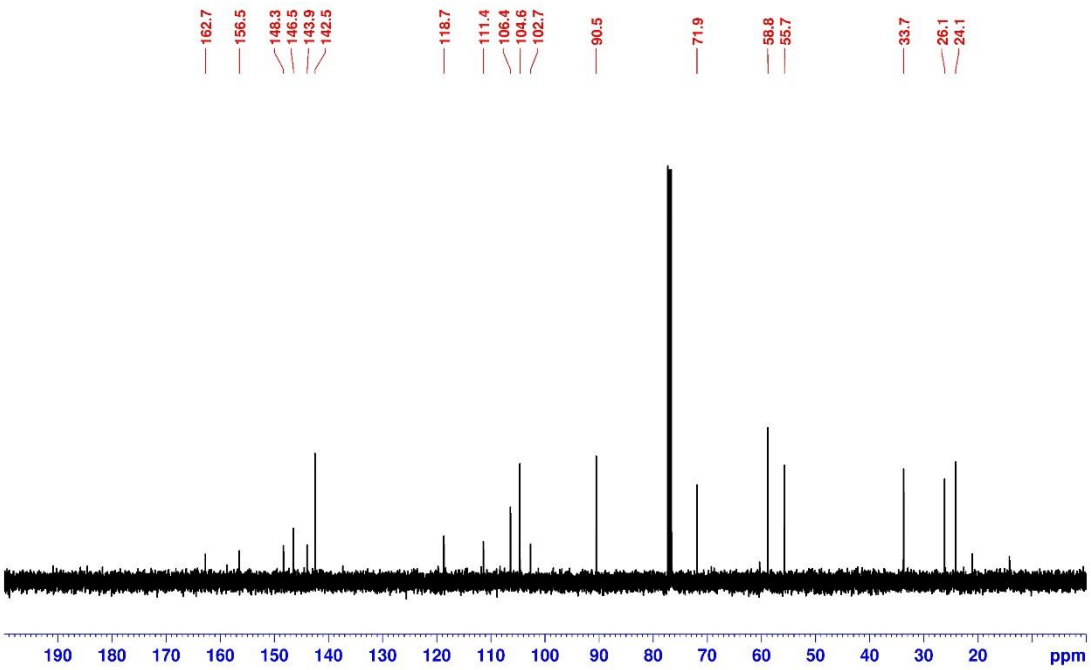
O(1)-C(2)-C(4)-C(5)	O(16)-C(17)-C(18)-C(19)
C(2)-O(1)-C(15)-C(6)	C(17)-C(18)-C(19)-C(20)
C(2)-O(1)-C(15)-C(12)	C(17)-C(18)-C(19)-C(21)
C(2)-C(4)-C(5)-C(6)	1.2(4)
O(3)-C(2)-C(4)-C(5)	178.8(2)
C(4)-C(5)-C(6)-C(7)	177.4(2)
C(4)-C(5)-C(6)-C(15)	0.5(3)
C(5)-C(6)-C(7)-C(8)	-176.5(2)
C(5)-C(6)-C(15)-O(1)	-2.4(3)
C(5)-C(6)-C(15)-C(12)	175.8(2)
C(6)-C(7)-C(8)-O(9)	178.3(2)
C(6)-C(7)-C(8)-C(11)	0.2(3)
C(7)-C(6)-C(15)-O(1)	-179.44(19)
C(7)-C(6)-C(15)-C(12)	-1.2(3)
C(7)-C(8)-O(9)-C(10)	-17.0(3)
C(7)-C(8)-C(11)-C(12)	0.1(3)
C(7)-C(8)-C(11)-O(16)	174.4(2)
C(8)-C(11)-C(12)-O(13)	177.9(2)
C(8)-C(11)-C(12)-C(15)	-1.0(3)
C(8)-C(11)-O(16)-C(17)	81.3(3)
O(9)-C(8)-C(11)-C(12)	-178.2(2)
O(9)-C(8)-C(11)-O(16)	-3.8(3)
C(11)-C(8)-O(9)-C(10)	161.2(2)
C(11)-C(12)-O(13)-C(14)	-79.3(3)
C(11)-C(12)-C(15)-O(1)	179.82(19)
C(11)-C(12)-C(15)-C(6)	1.5(3)
C(11)-O(16)-C(17)-C(18)	166.2(3)
C(12)-C(11)-O(16)-C(17)	-104.3(3)
O(13)-C(12)-C(15)-O(1)	0.9(3)
O(13)-C(12)-C(15)-C(6)	-177.33(19)
C(15)-O(1)-C(2)-O(3)	179.30(19)
C(15)-O(1)-C(2)-C(4)	-0.8(3)
C(15)-C(6)-C(7)-C(8)	0.3(3)
C(15)-C(12)-O(13)-C(14)	99.6(3)
O(16)-C(11)-C(12)-O(13)	3.4(3)
O(16)-C(11)-C(12)-C(15)	-175.68(18)

Table 8. Hydrogen bonds for TCD415 [Å and °].

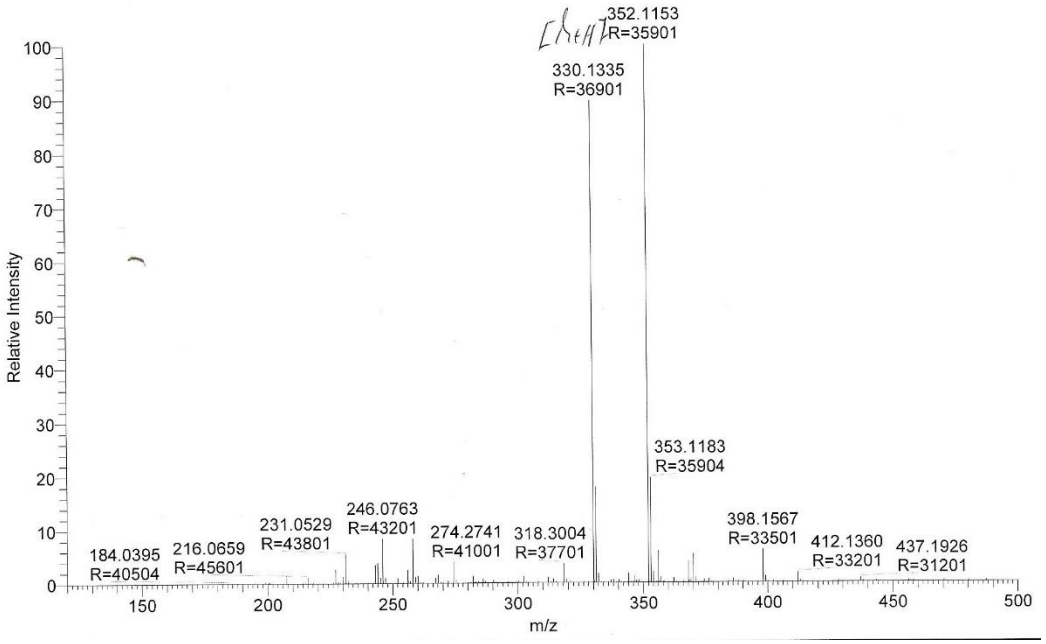
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(14)-H(14C)...O(16)	0.96	2.63	3.133(4)	113



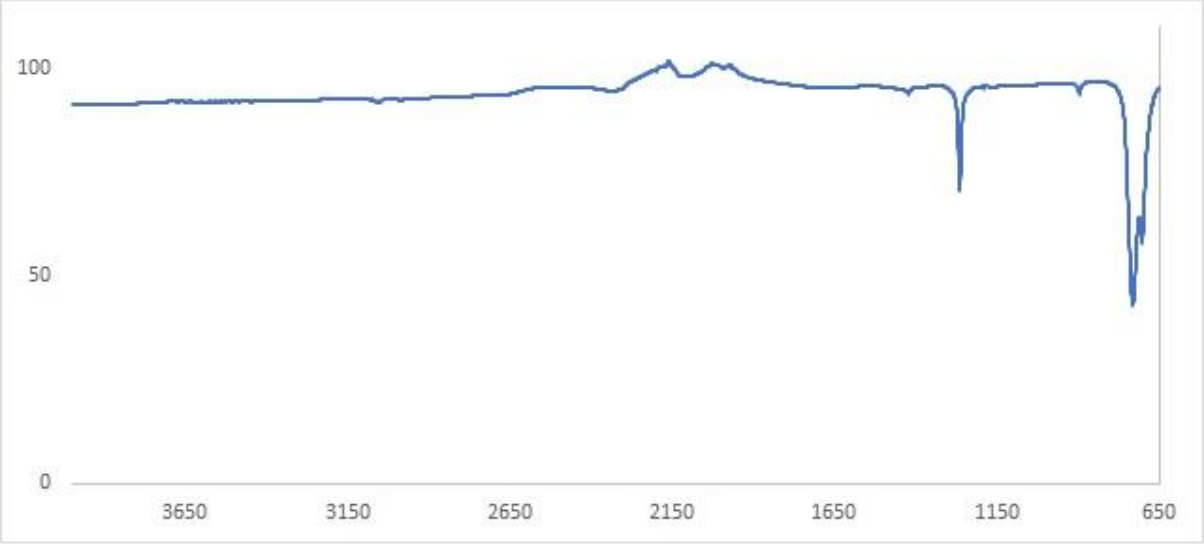
A. 26 ^{1}H NMR spectrum of **(2.07)**



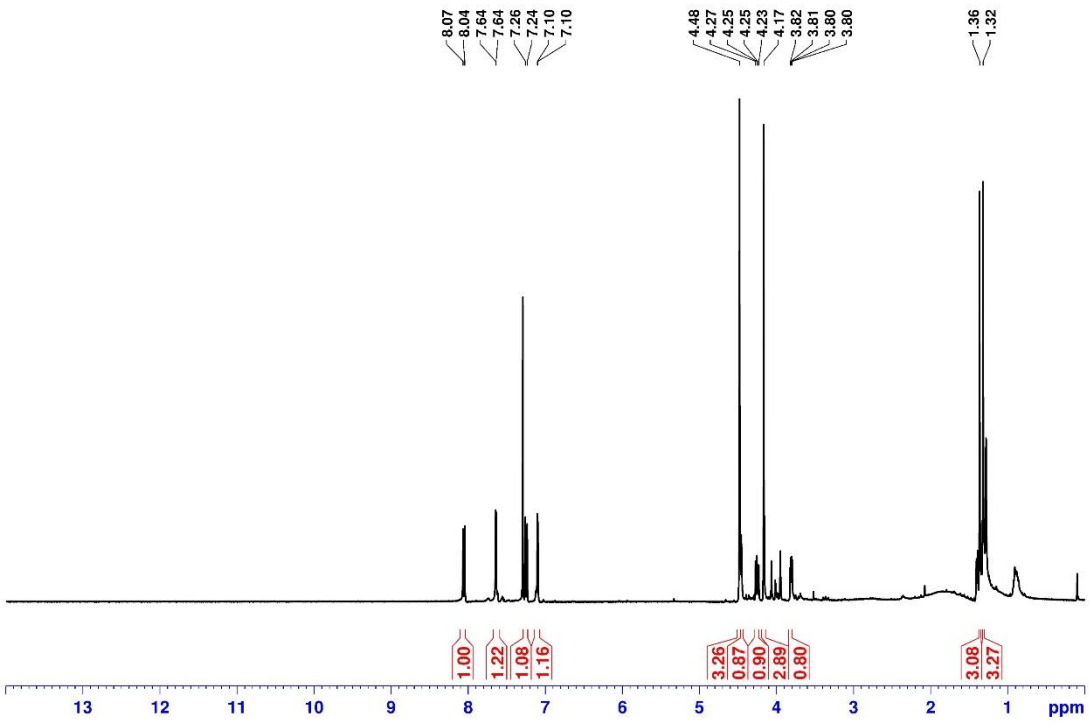
A. 27 ^{13}C NMR spectrum of **(2.07)**



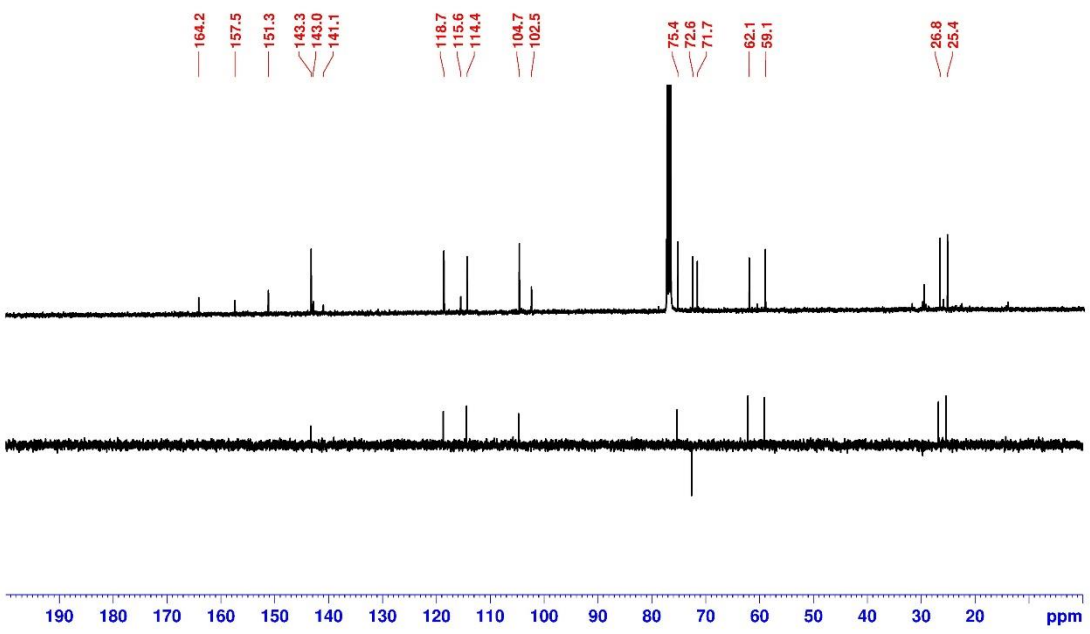
A. 28 ESI-HRMS of **(2.07)**, positive mode m/z 330.1335 $[M+H]^+$



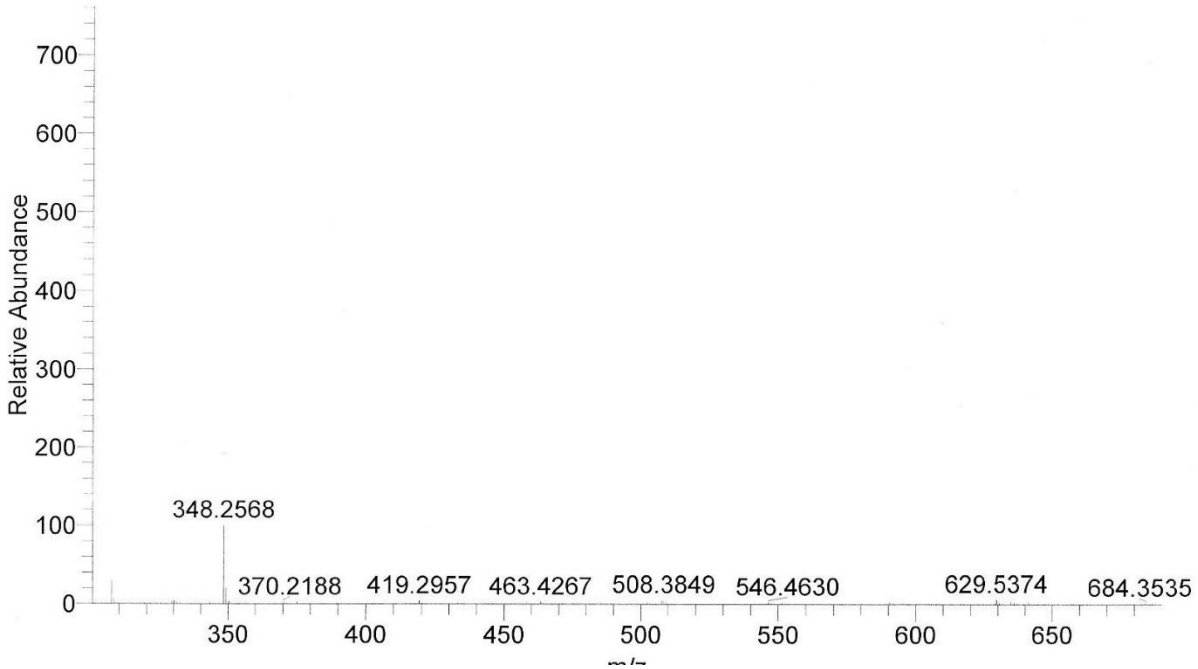
A. 29 IR spectrum of **(2.07)**



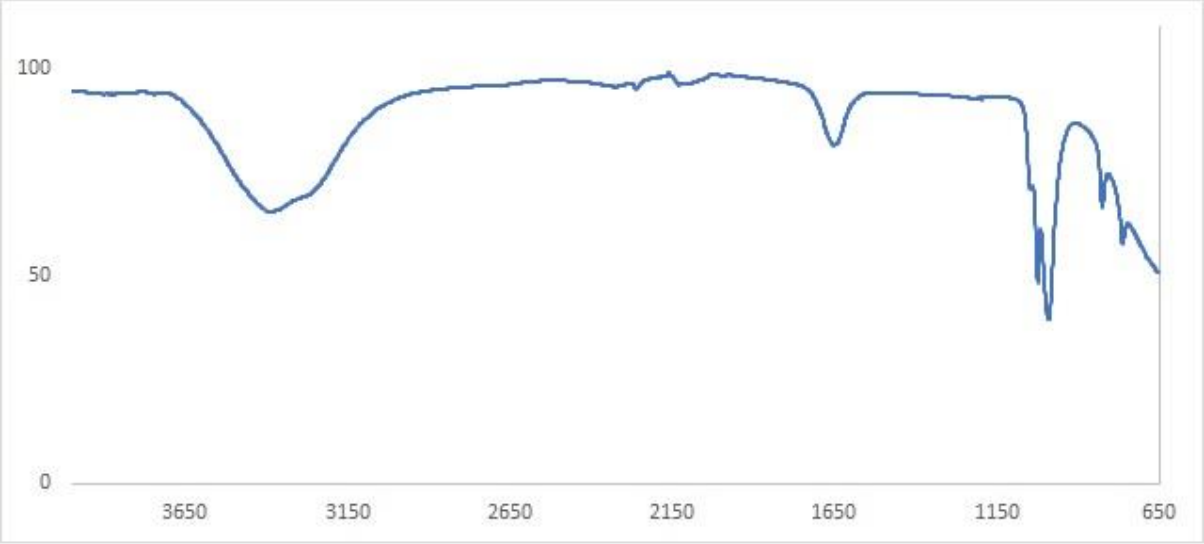
A. 30 ^{1}H NMR spectrum of **(2.08)**



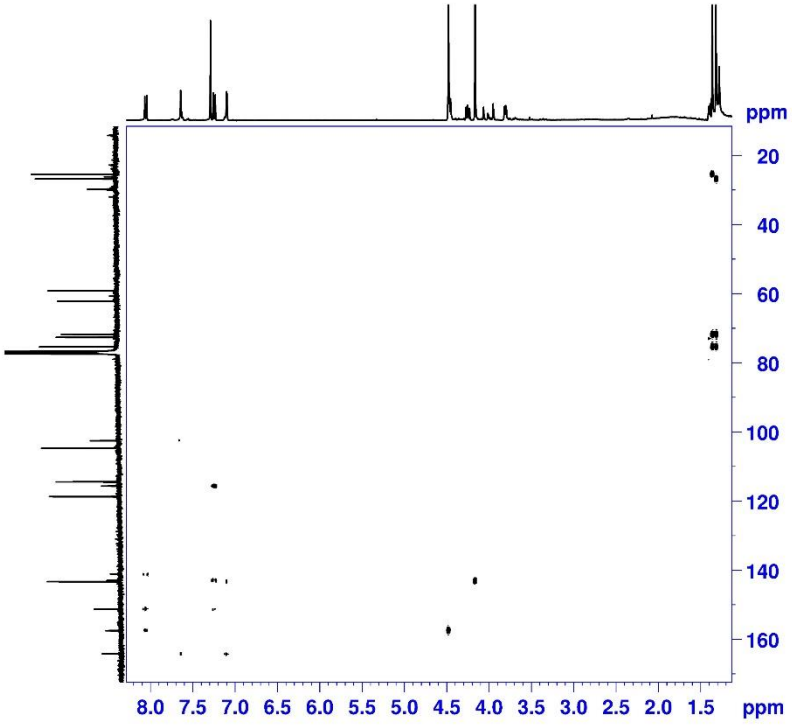
A. 31 ^{13}C NMR spectrum of **(2.08)**



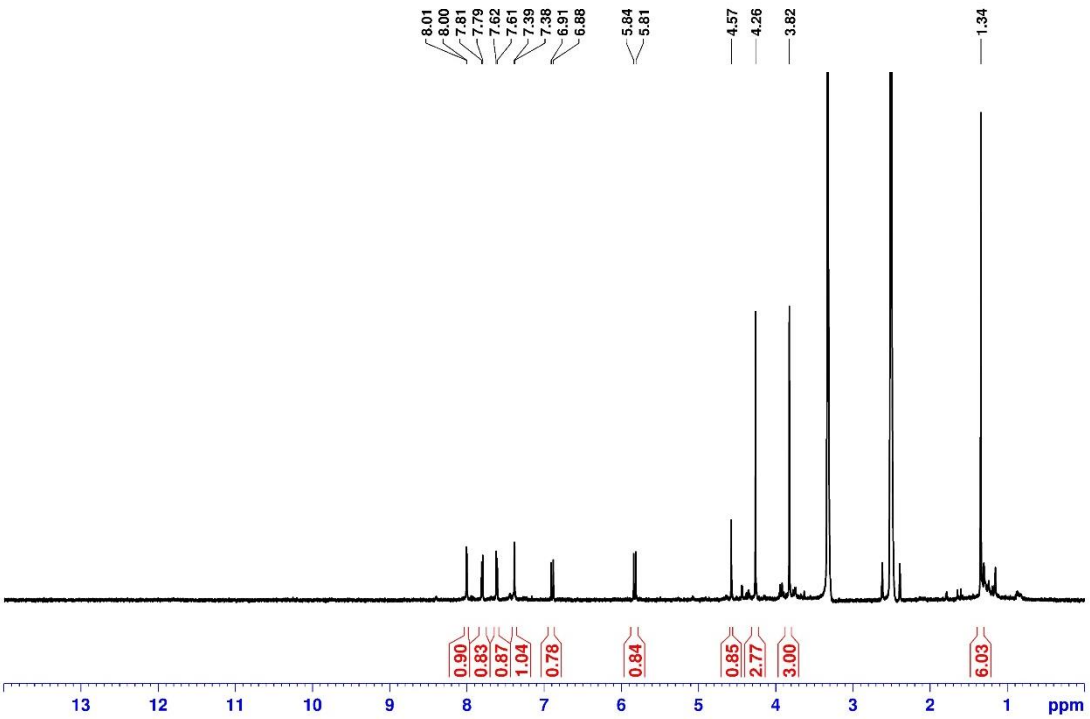
A. 32 ESI-HRMS of **(2.08)**, positive mode m/z 348.2568 $[M+H]^+$



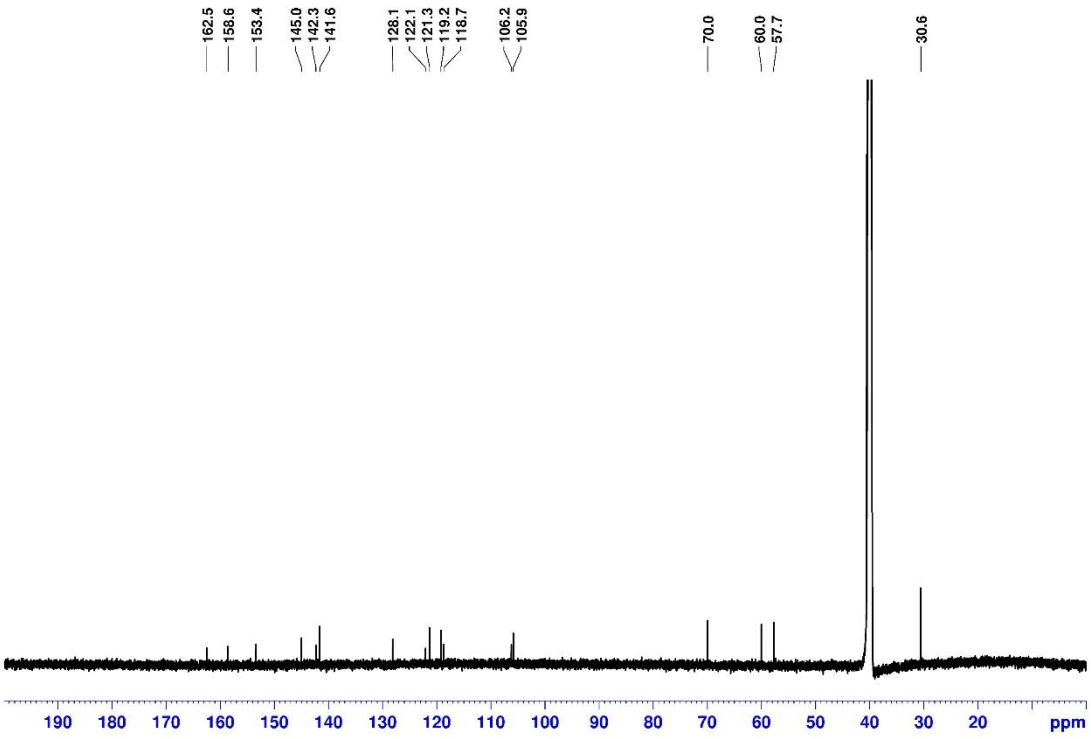
A. 33 IR spectrum of **(2.08)**



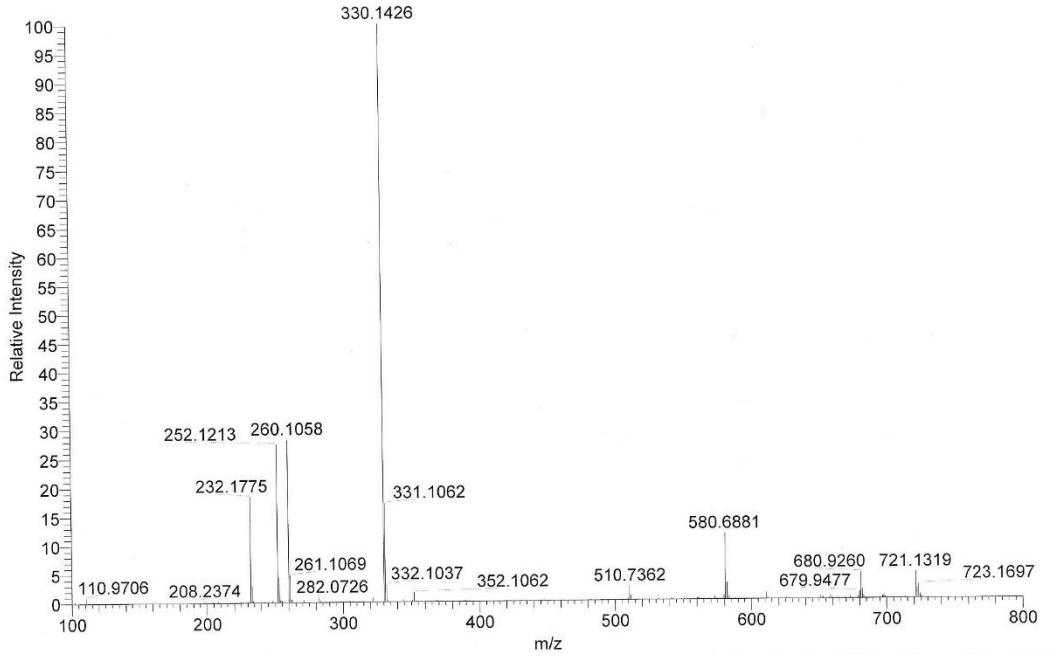
A. 34 HMBC spectrum of **(2.08)**



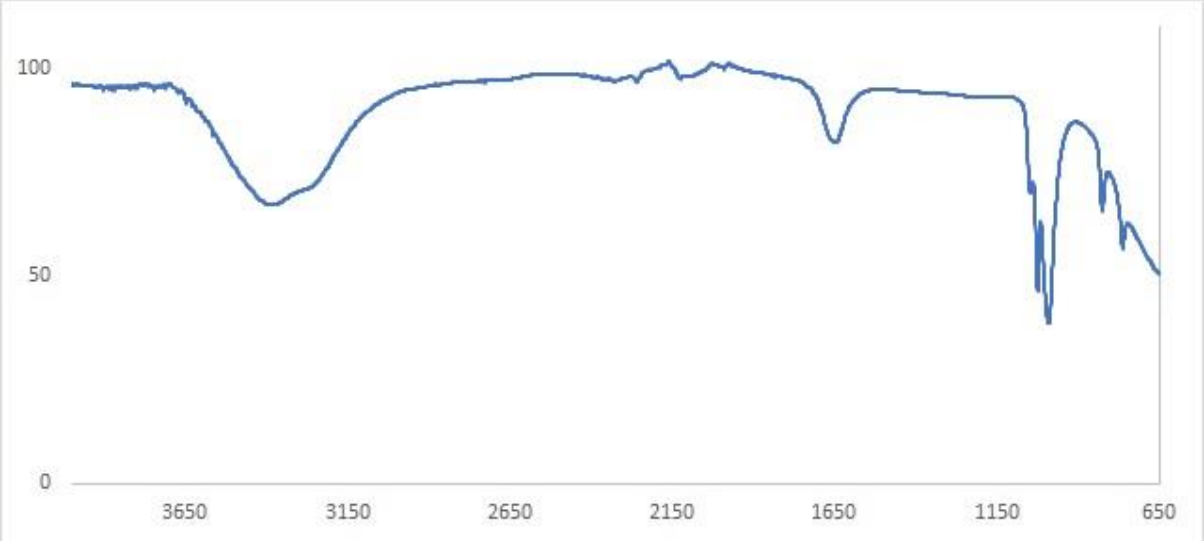
A. 35 ^{1}H NMR spectrum of **(2.09)**



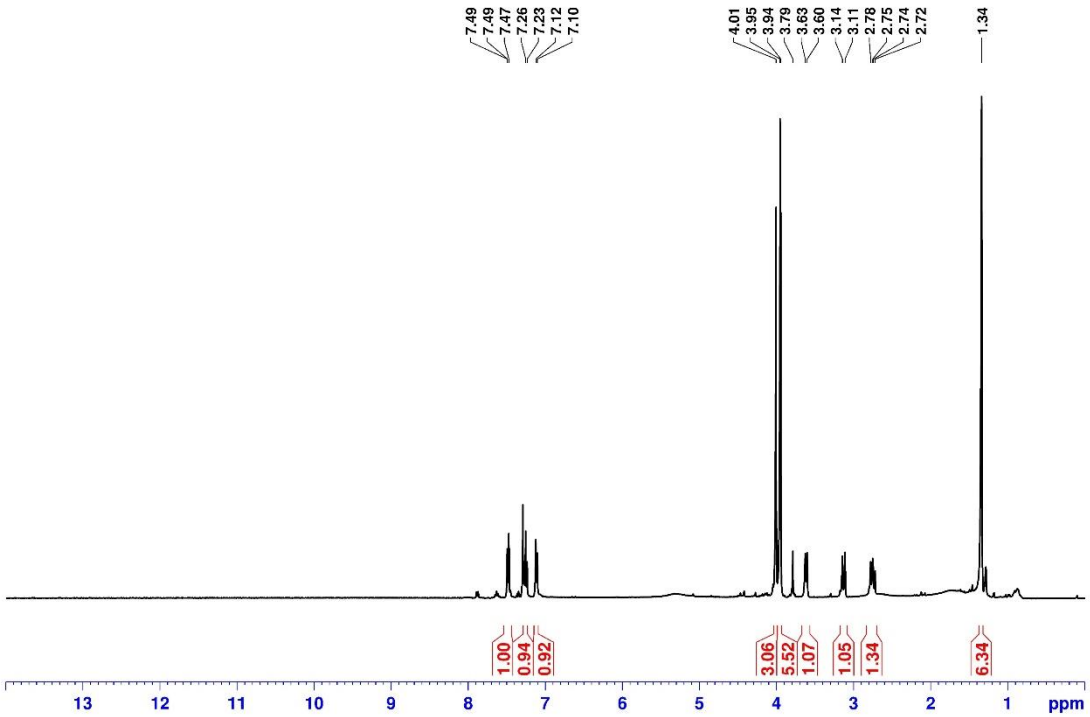
A. 36 ^{13}C NMR spectrum of **(2.09)**



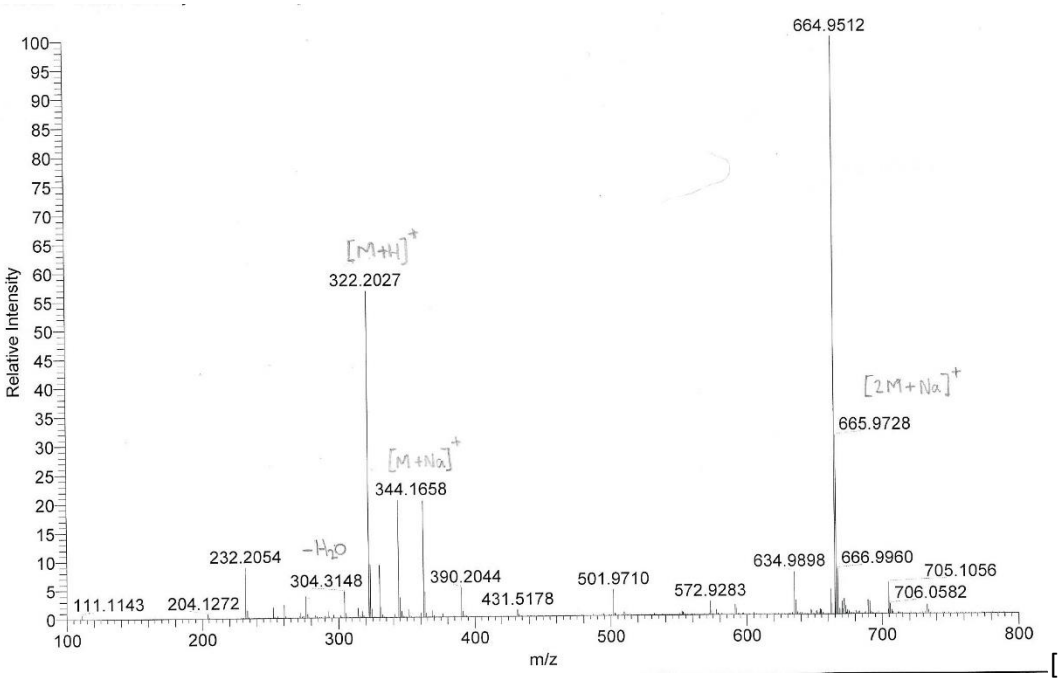
A. 37 ESI-HRMS of **(2.09)**, positive mode m/z 330.1426 $[M+H]^+$



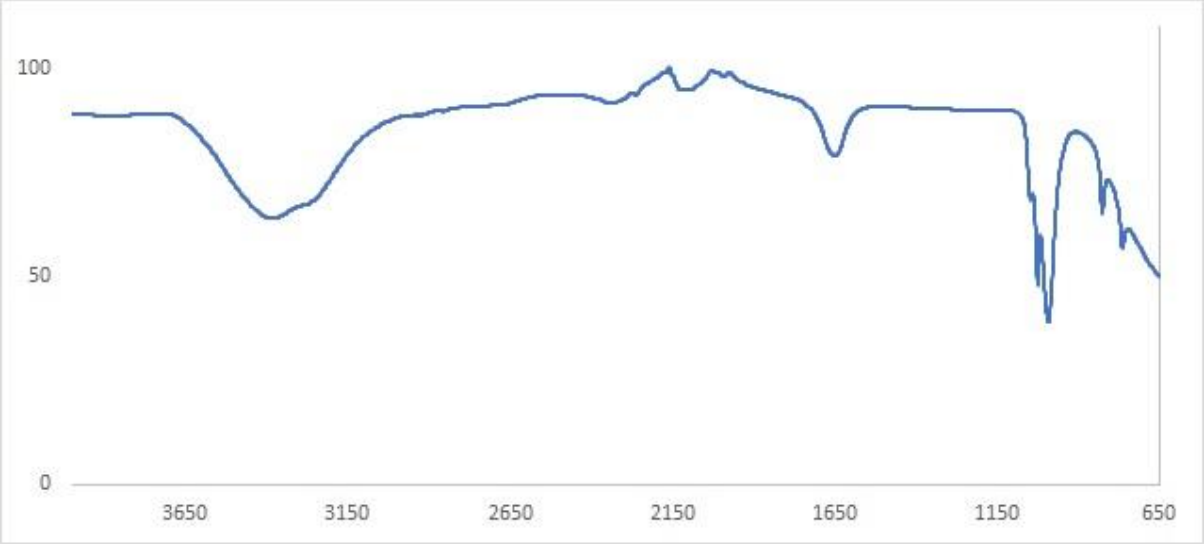
A. 38 IR spectrum of **(2.09)**



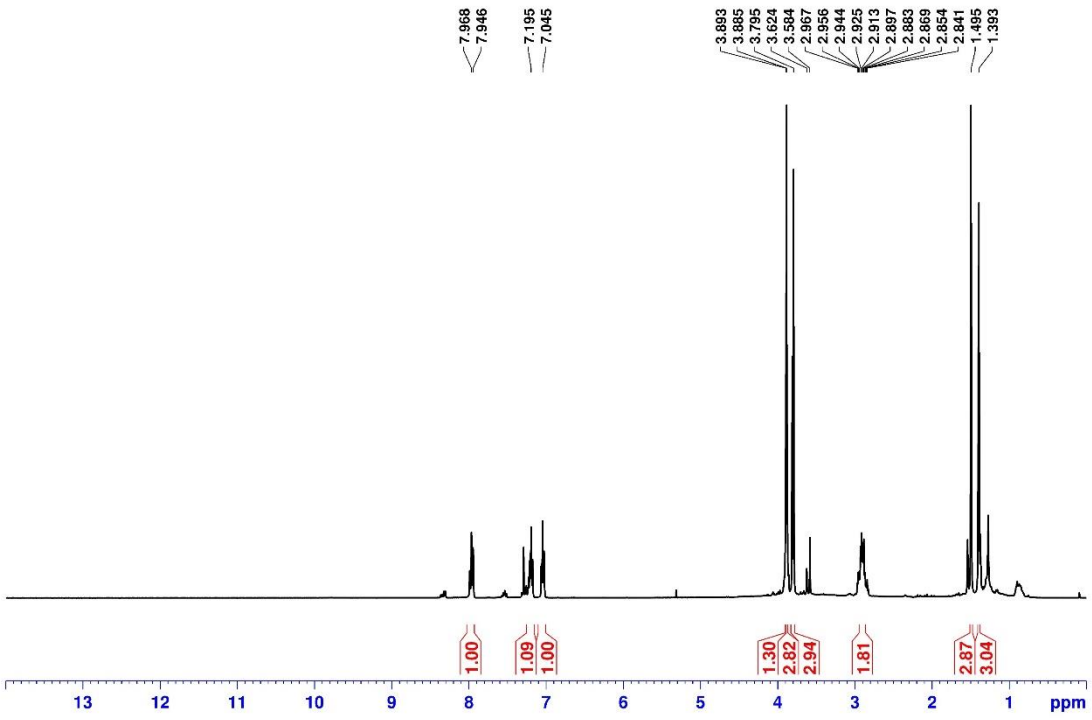
A. 39 ^{1}H NMR spectrum of **(2.10)**



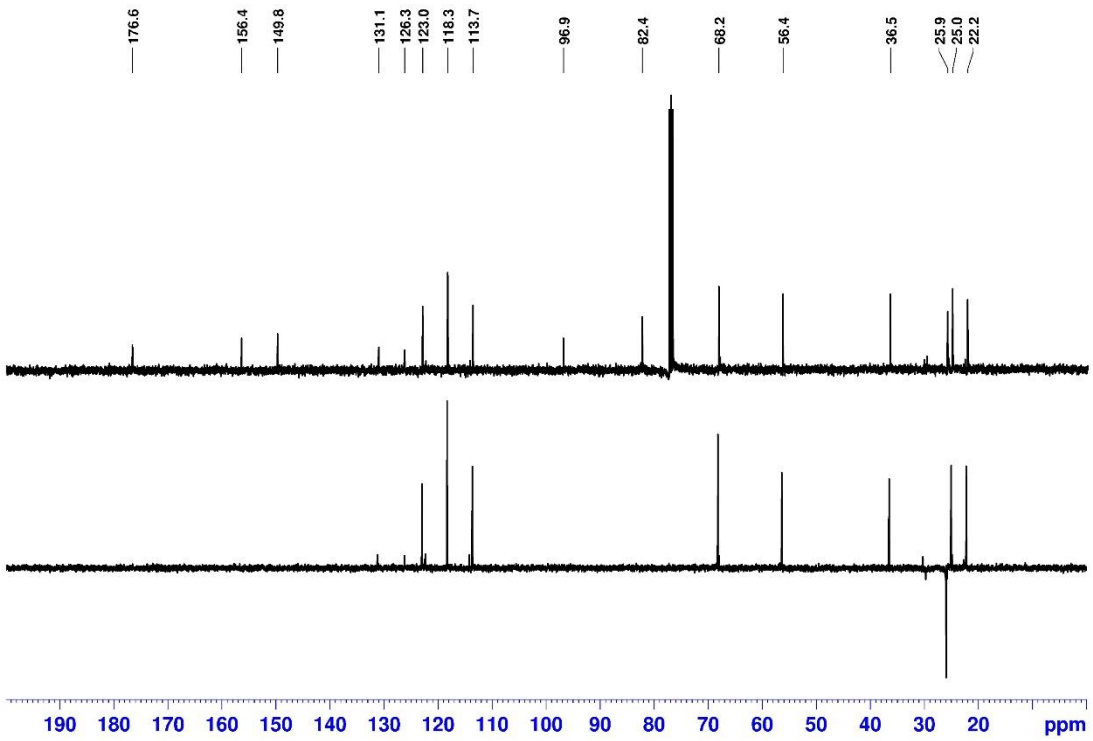
A. 40 ESI-HRMS of **(2.10)**, positive mode m/z 322.2027 $[M+H]^{+}$



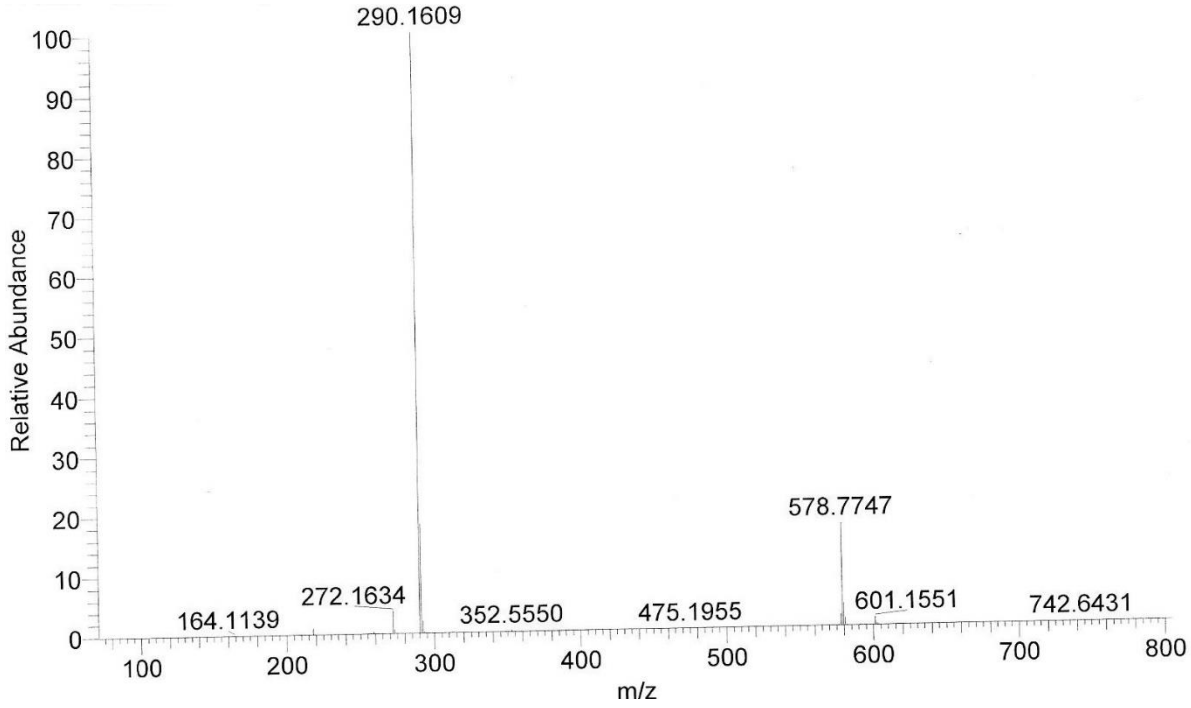
A. 41 IR spectrum of **(2.10)**



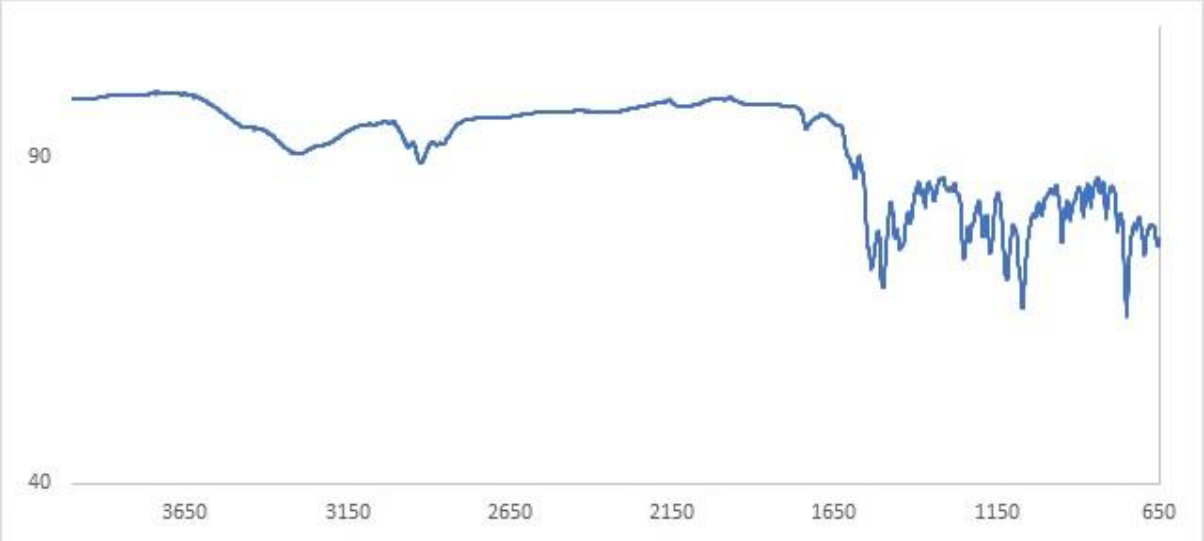
A. 42 ^{1}H NMR spectrum of **(2.11)**



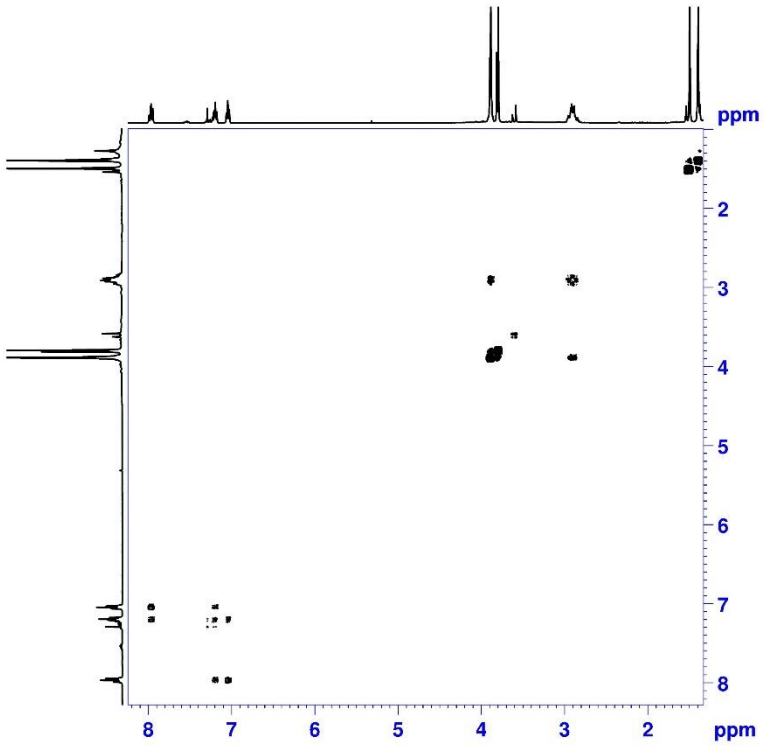
A. 43 ^{13}C NMR spectrum of **(2.11)**



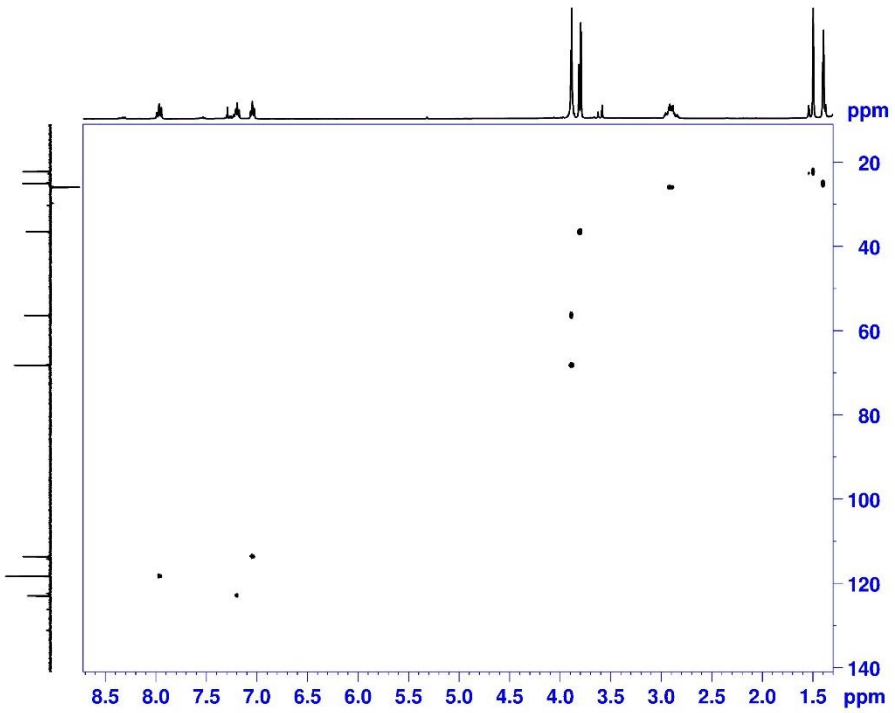
A. 44 ESI-HRMS of **(2.11)**, positive mode m/z 290.1609 $[M+H]^+$



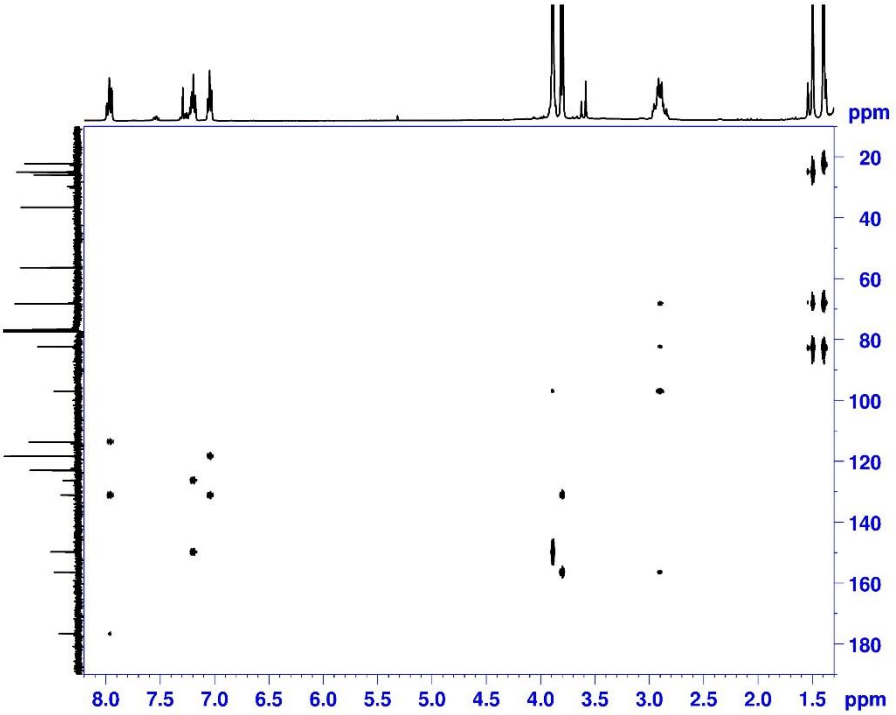
A. 45 IR spectrum of **(2.11)**



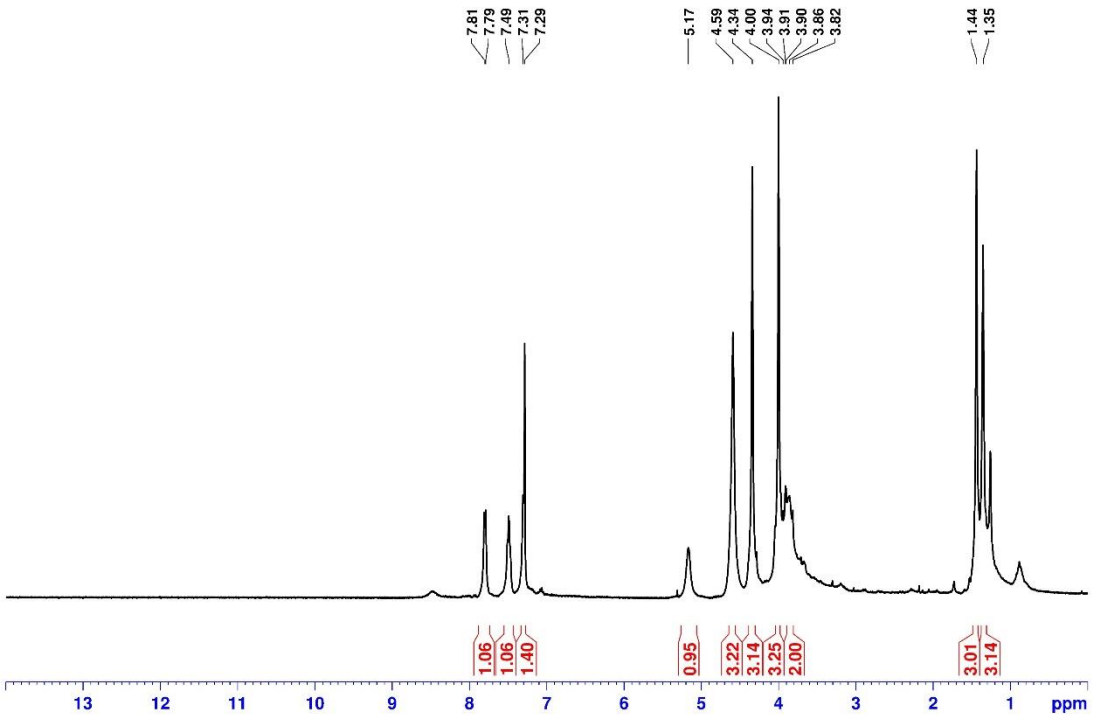
A. 46 ^{1}H-^{1}H COSY spectrum of **(2.11)**



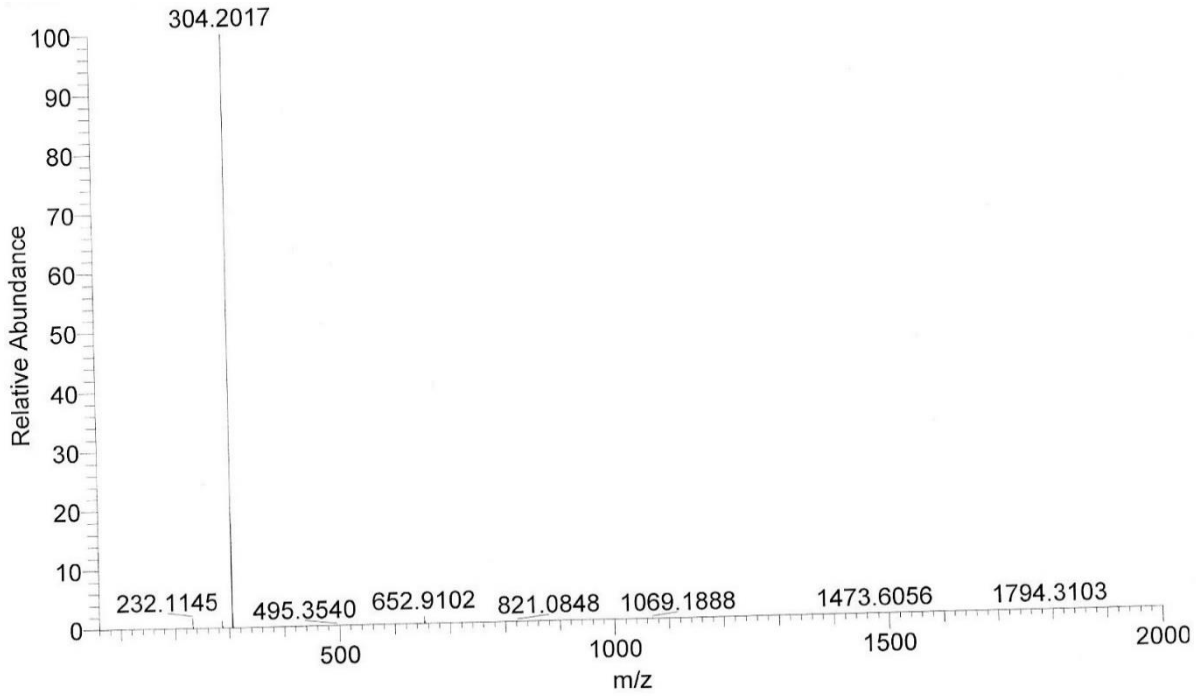
A. 47 HSQC spectrum of **(2.11)**



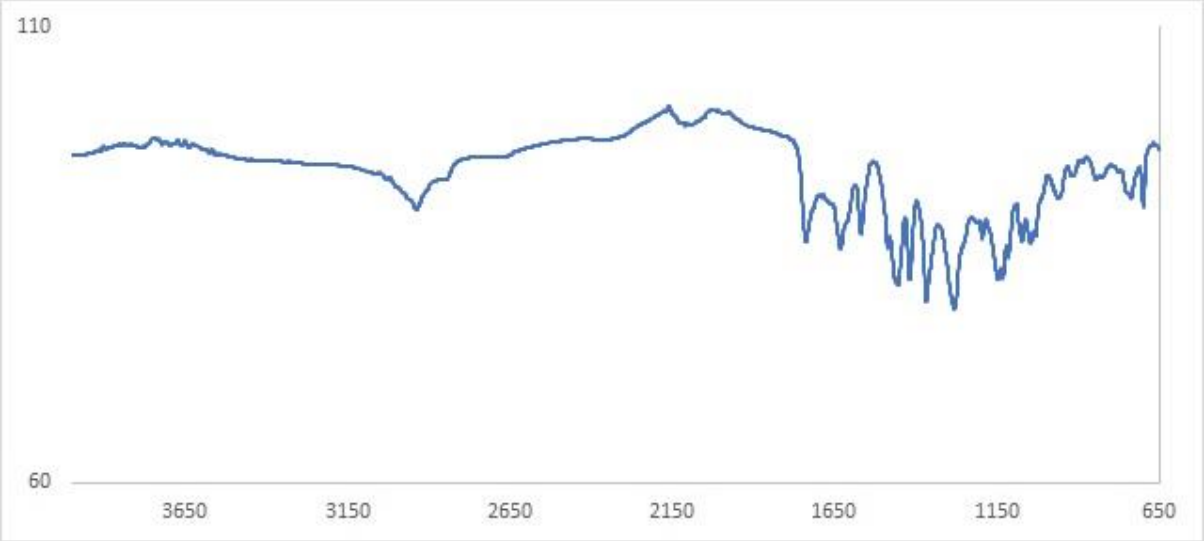
A. 48 HMBC spectrum of **(2.11)**



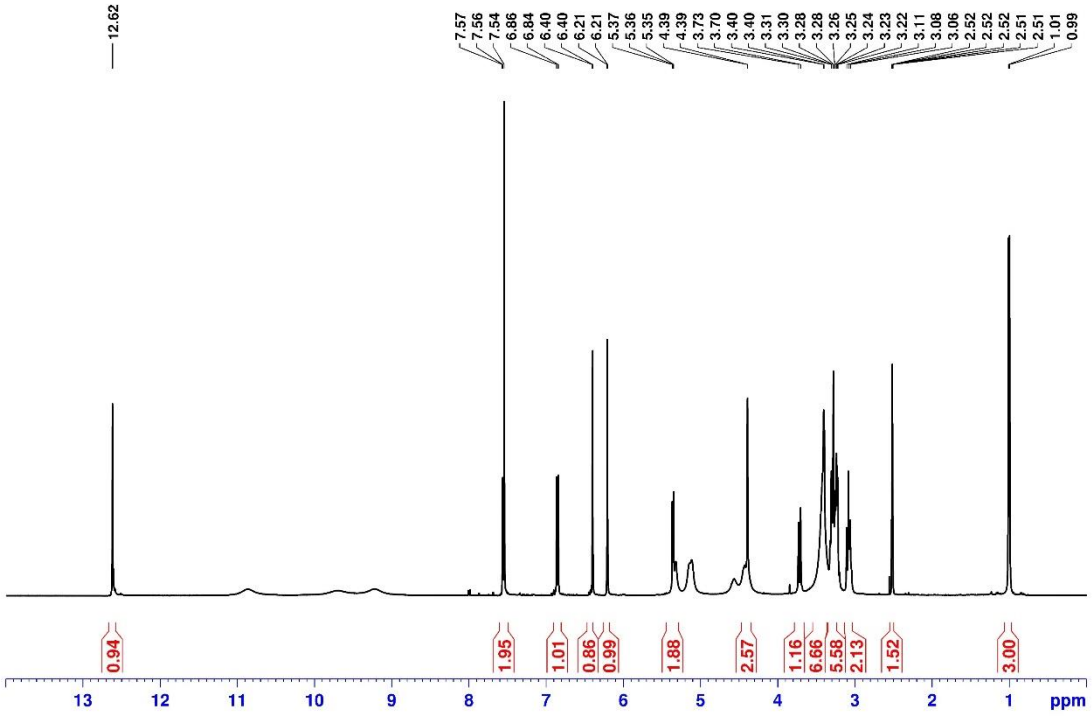
A. 49 ^{1}H NMR spectrum of **(2.12)**



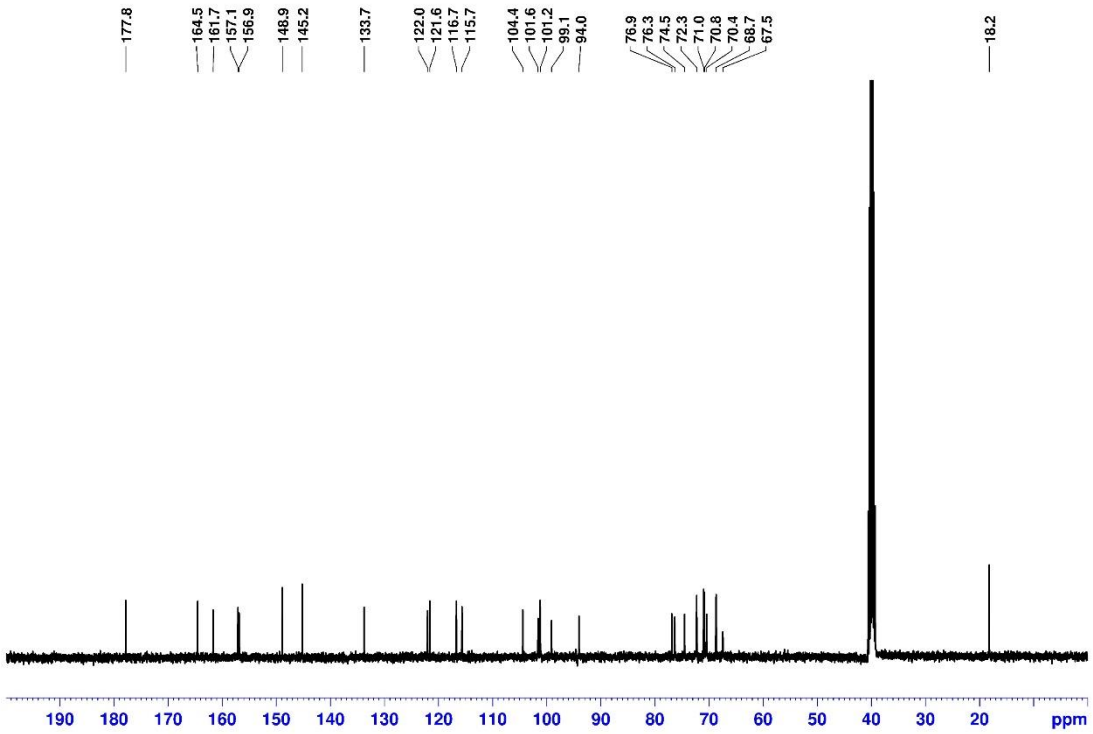
A. 50 ESI-HRMS of **(2.12)**, positive mode m/z 304.2017 [M+H]



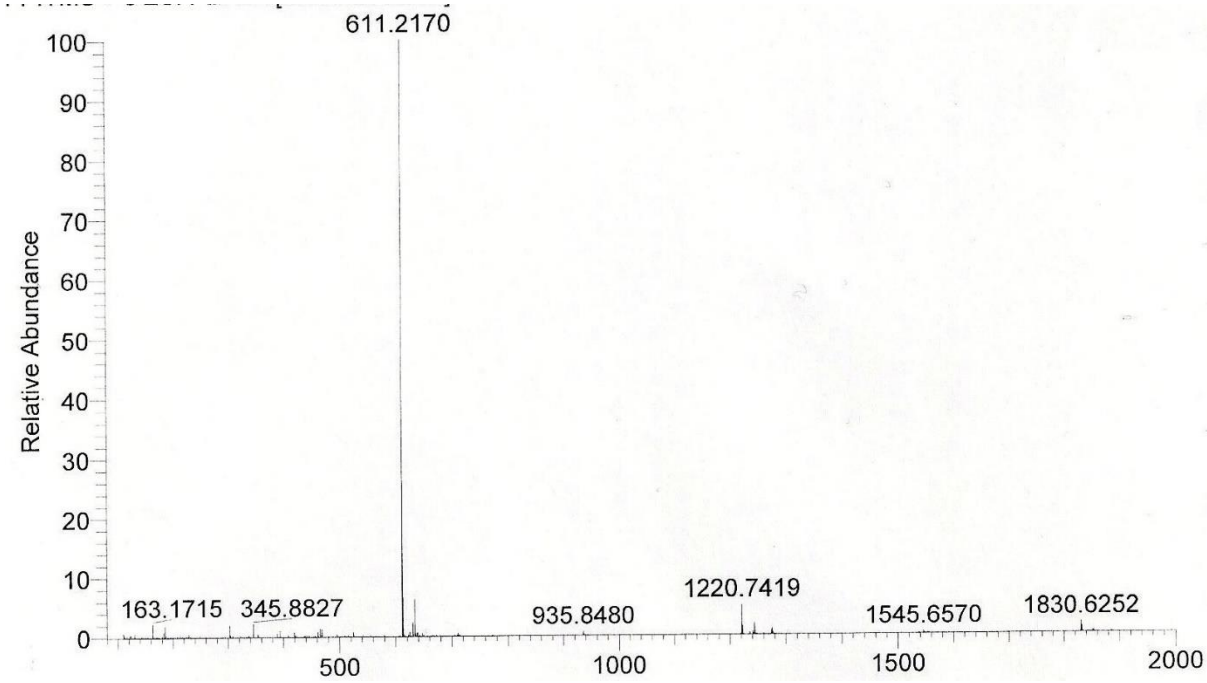
A. 51 IR spectrum of **(2.12)**



A. 52 ^{1}H NMR spectrum of **(2.13)**

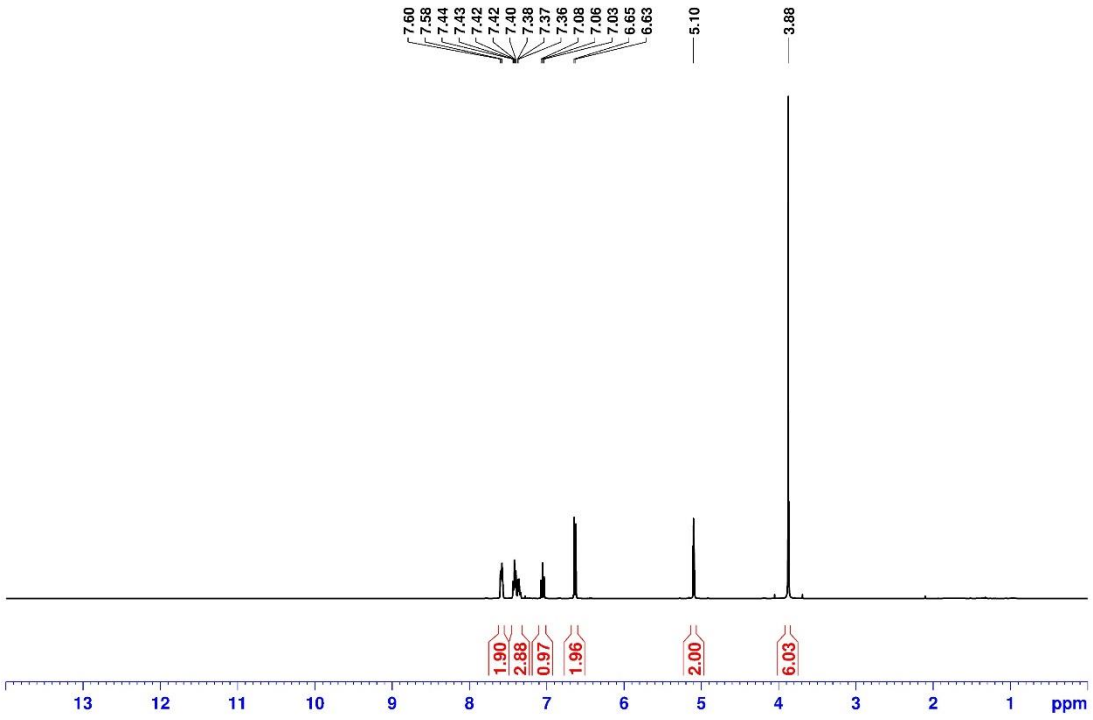


A. 53 ^{13}C NMR spectrum of **(2.13)**

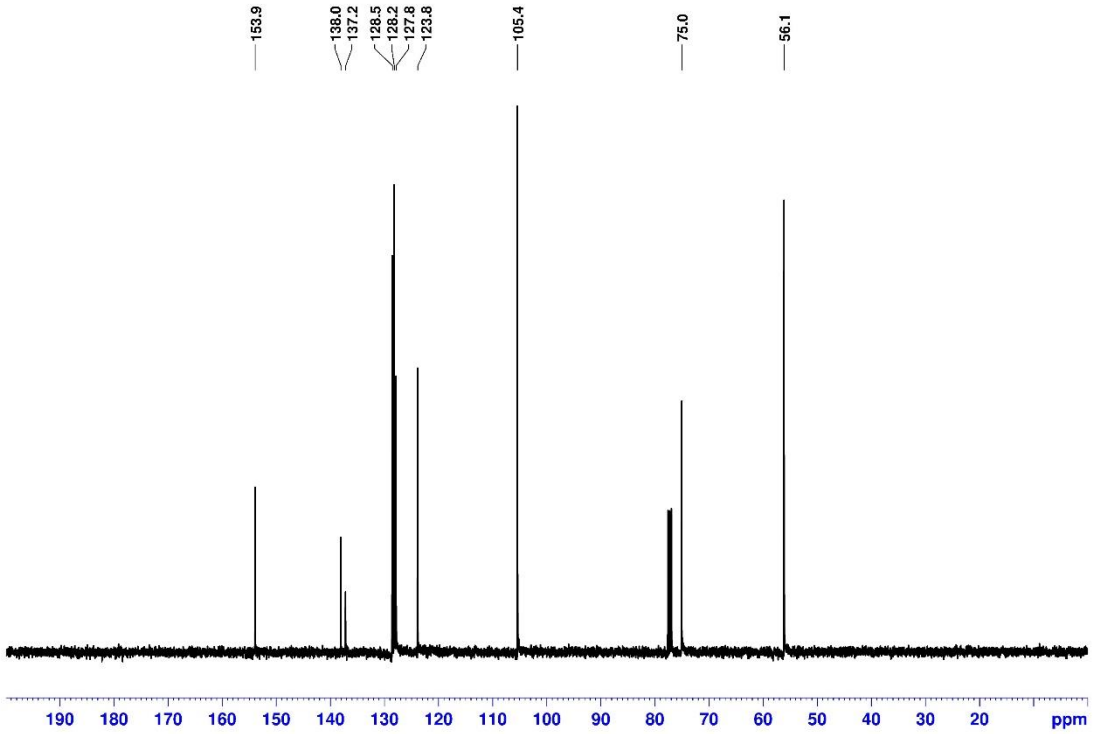


A. 54 ESI-HRMS of **(2.13)**, positive mode m/z 611.2170 $[M+H]^+$

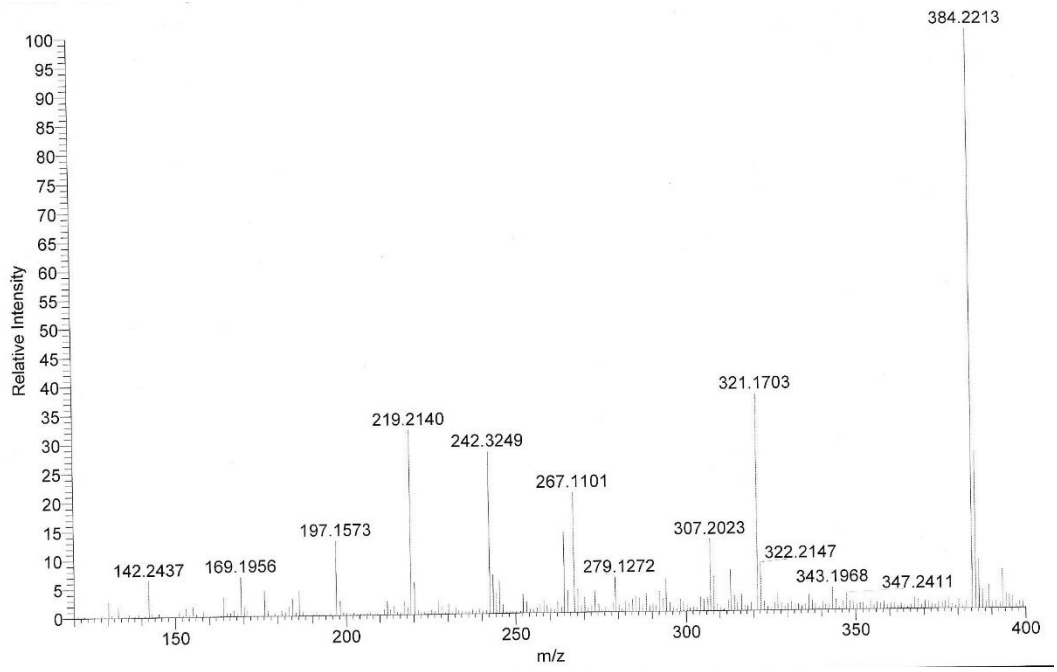
2. Spectroscopic Data of Chapter 5



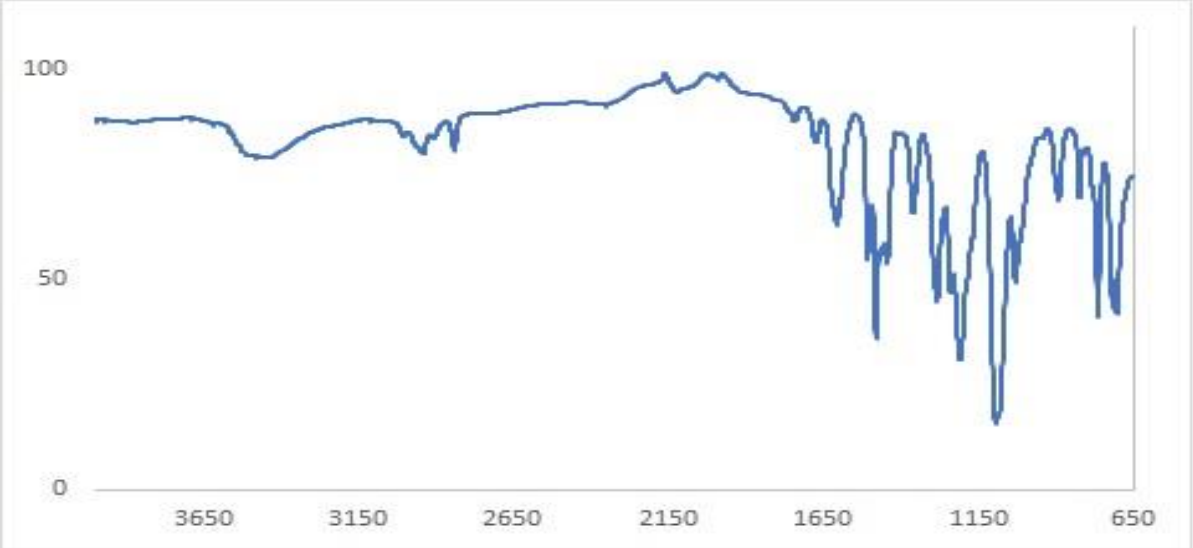
A. 55 ^{1}H NMR spectrum of **(4.02)**



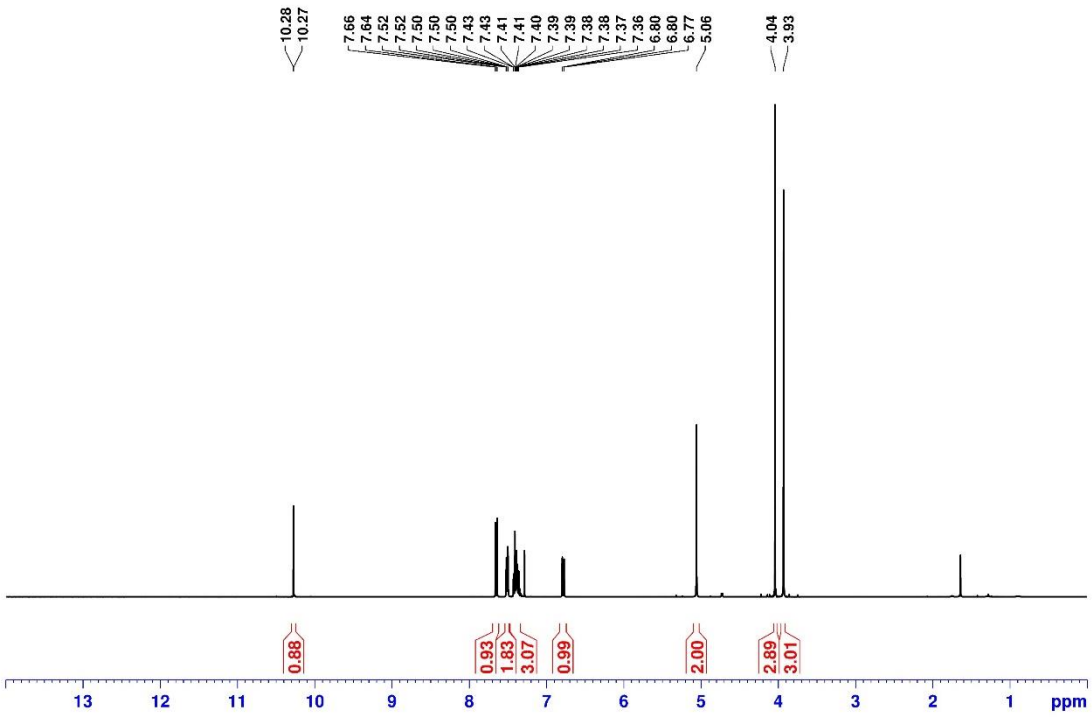
A. 56 ^{13}C NMR spectrum of **(4.02)**



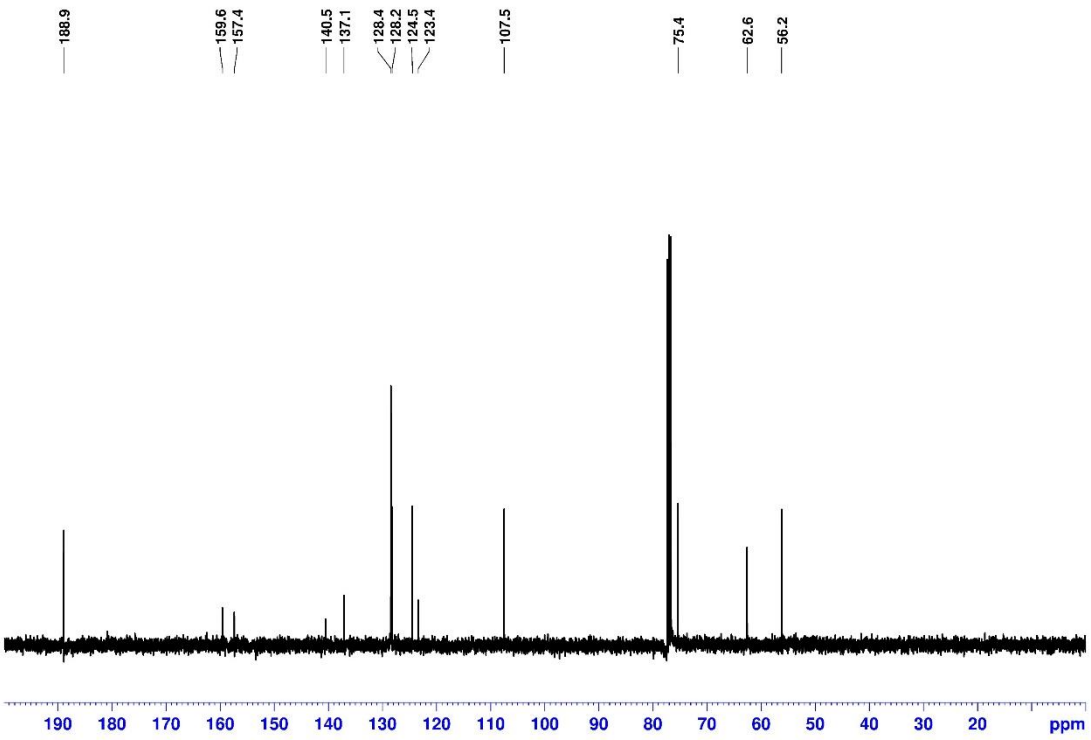
A. 57 ESI-MS of **(4.02)**, positive mode m/z 267 $[M+H]^+$



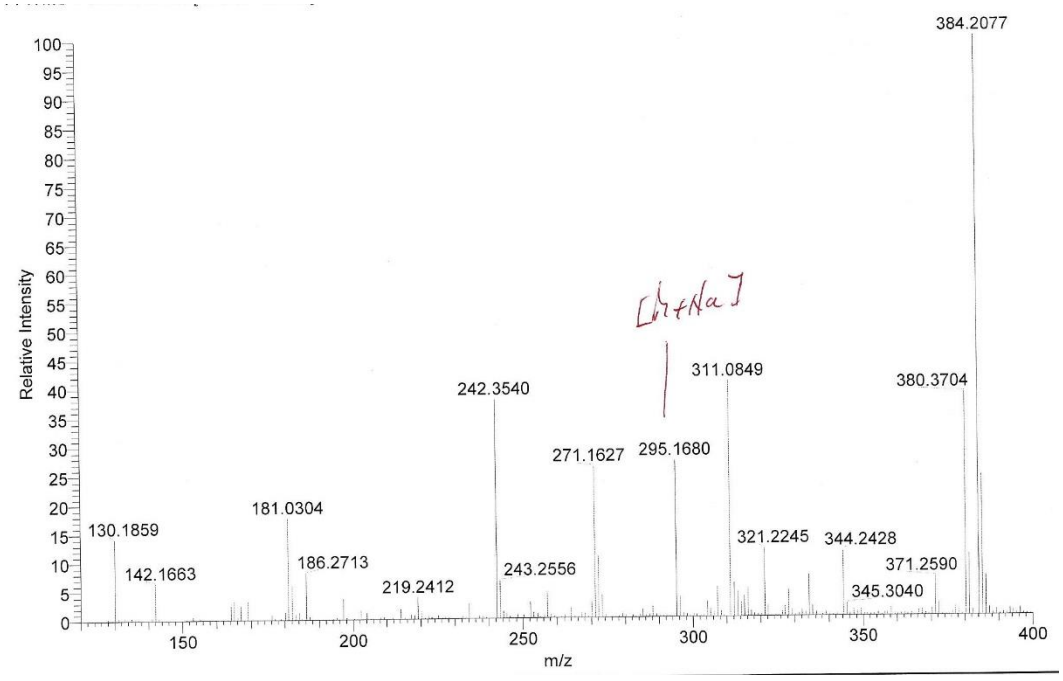
A. 58 IR spectrum of **(4.02)**



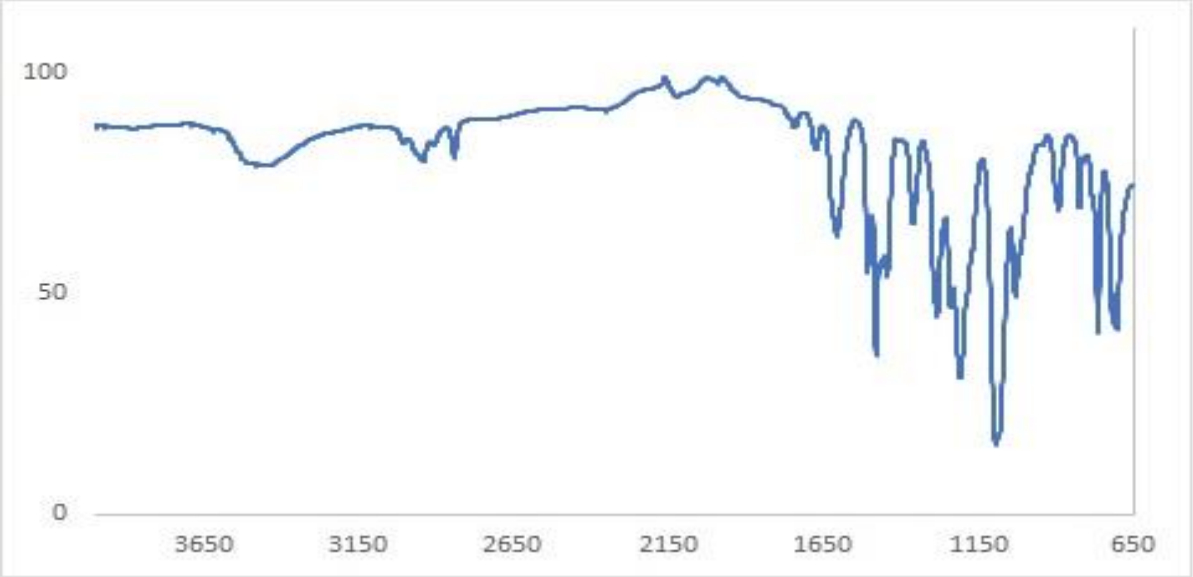
A. 59 ^{1}H NMR spectrum of **(4.03)**



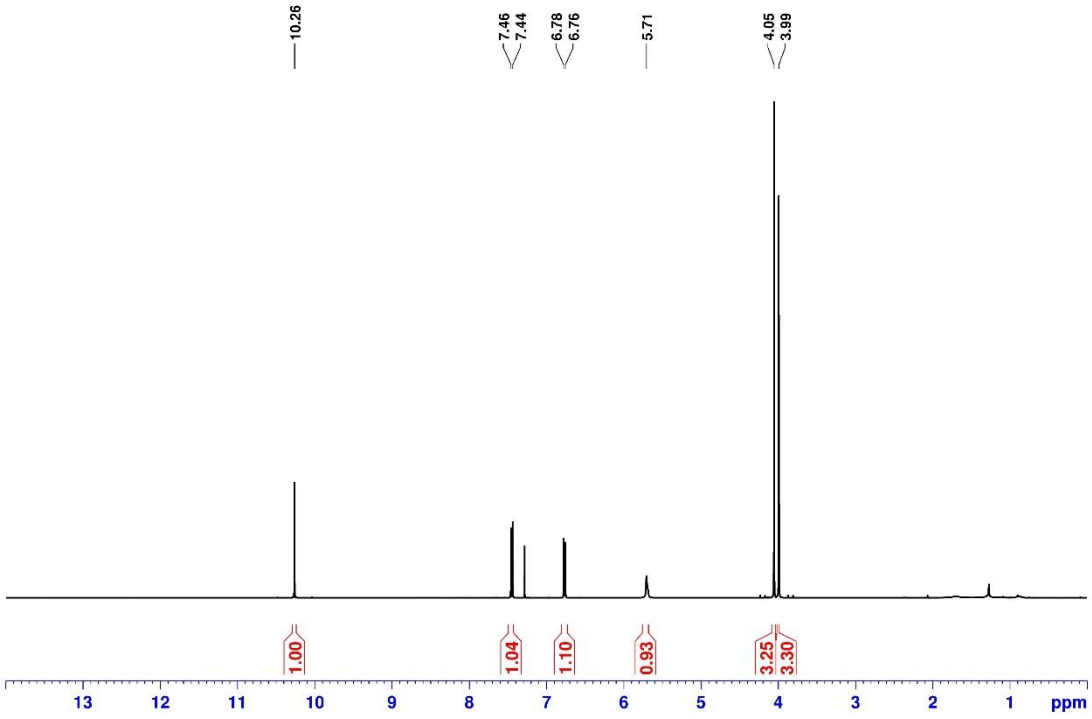
A. 60 ^{13}C NMR spectrum of **(4.03)**



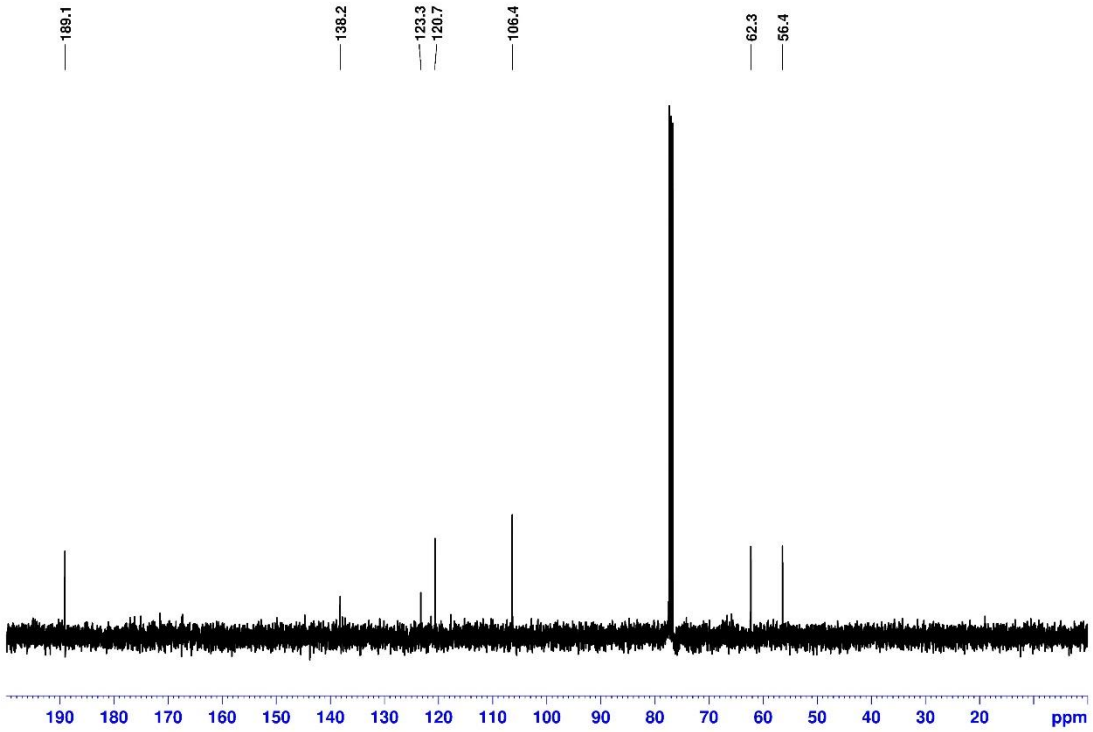
A. 61 ESI-MS of **(4.03)**, positive mode m/z 295 $[M+Na]^+$



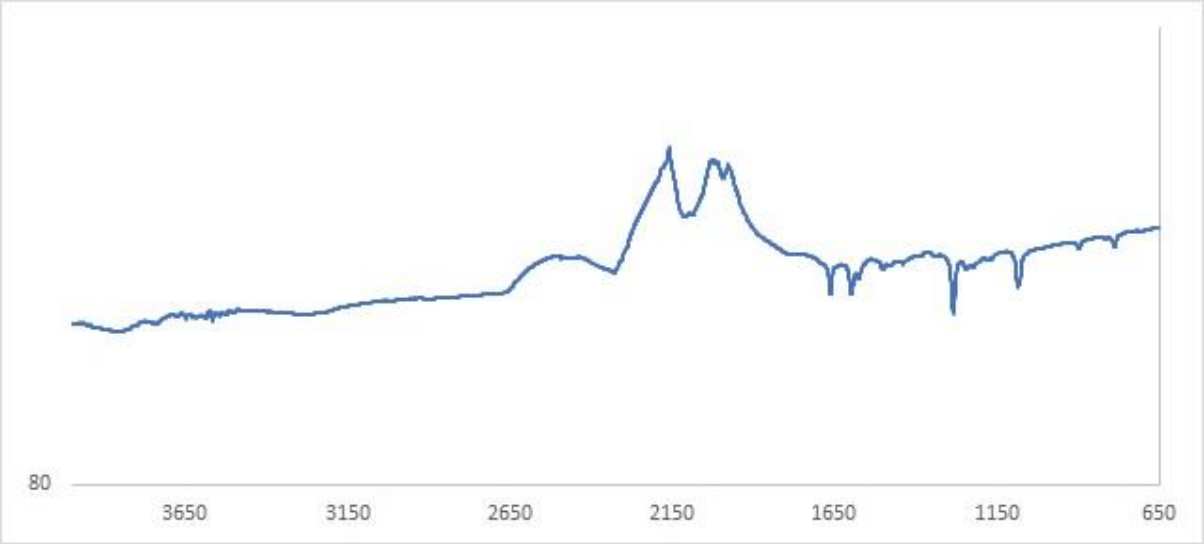
A. 62 IR spectrum of **(4.03)**



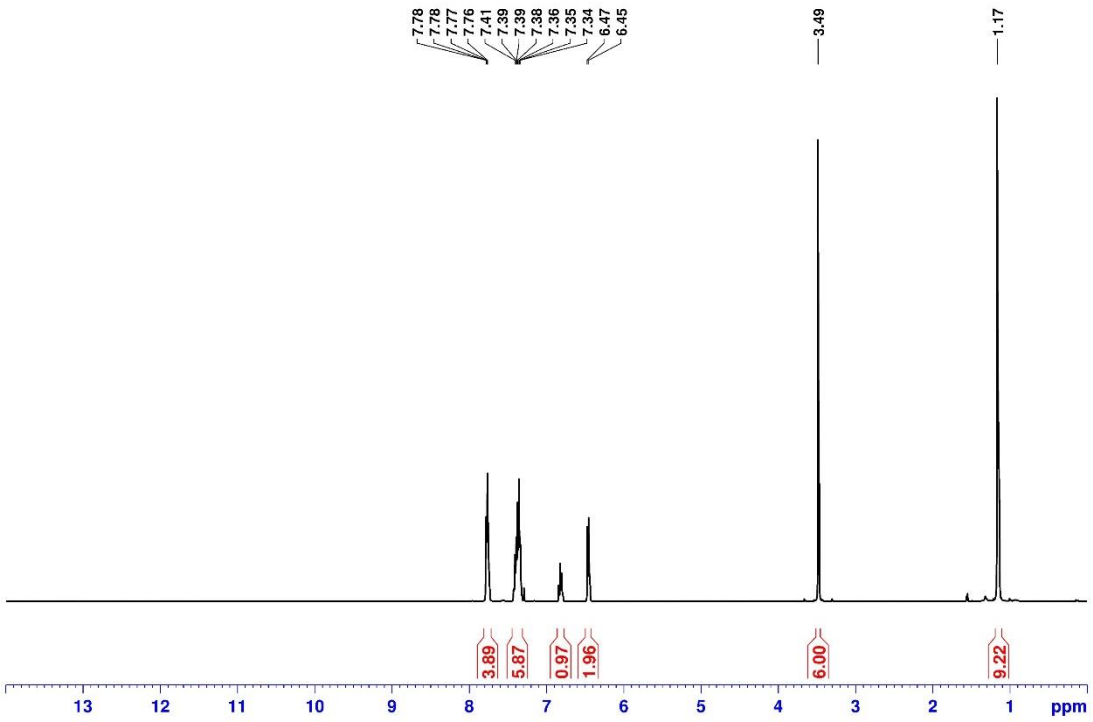
A. 63 ^{1}H NMR spectrum of **(4.04)**



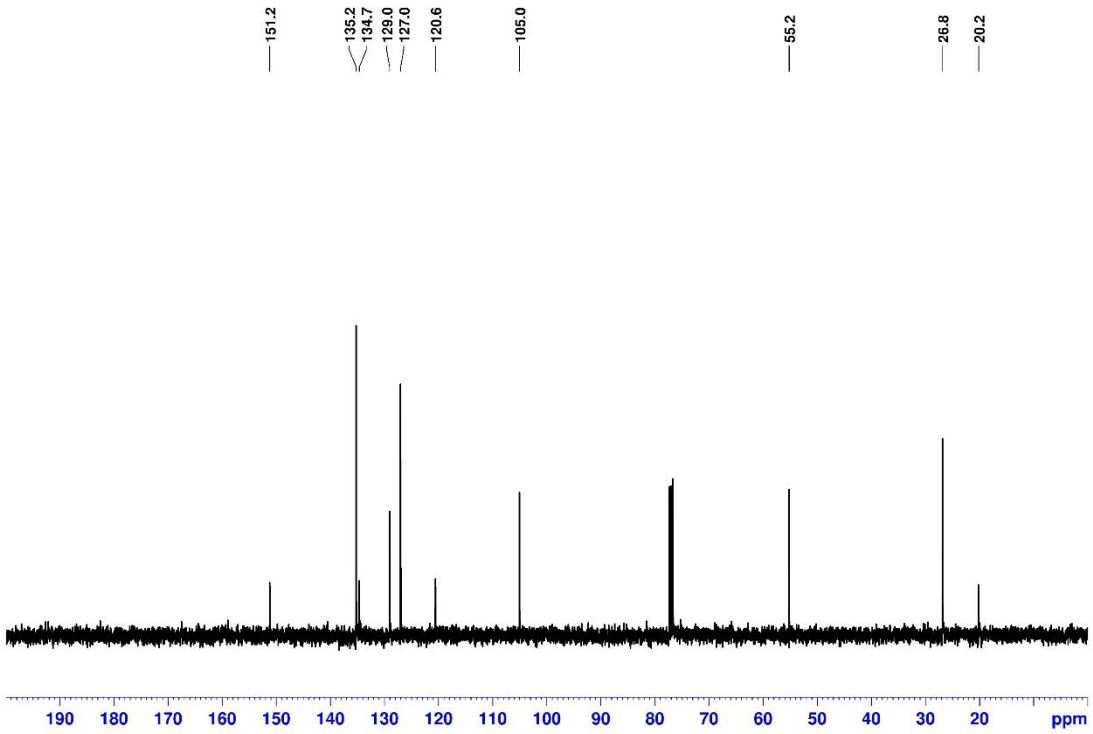
A. 64 ^{13}C NMR spectrum of **(4.04)**



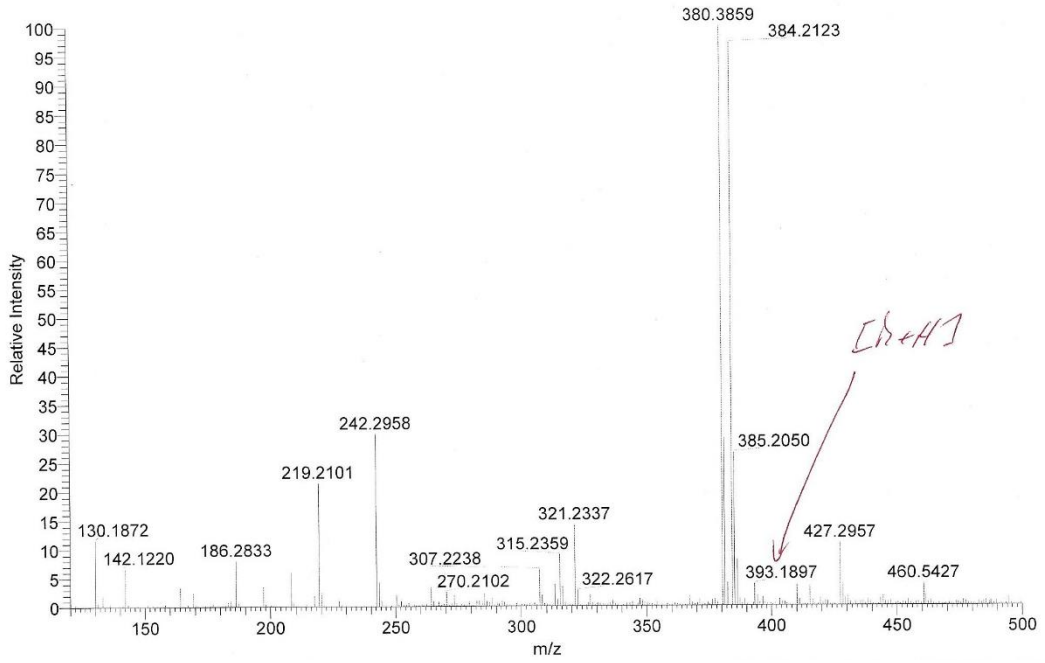
A. 65 IR spectrum of **(4.04)**



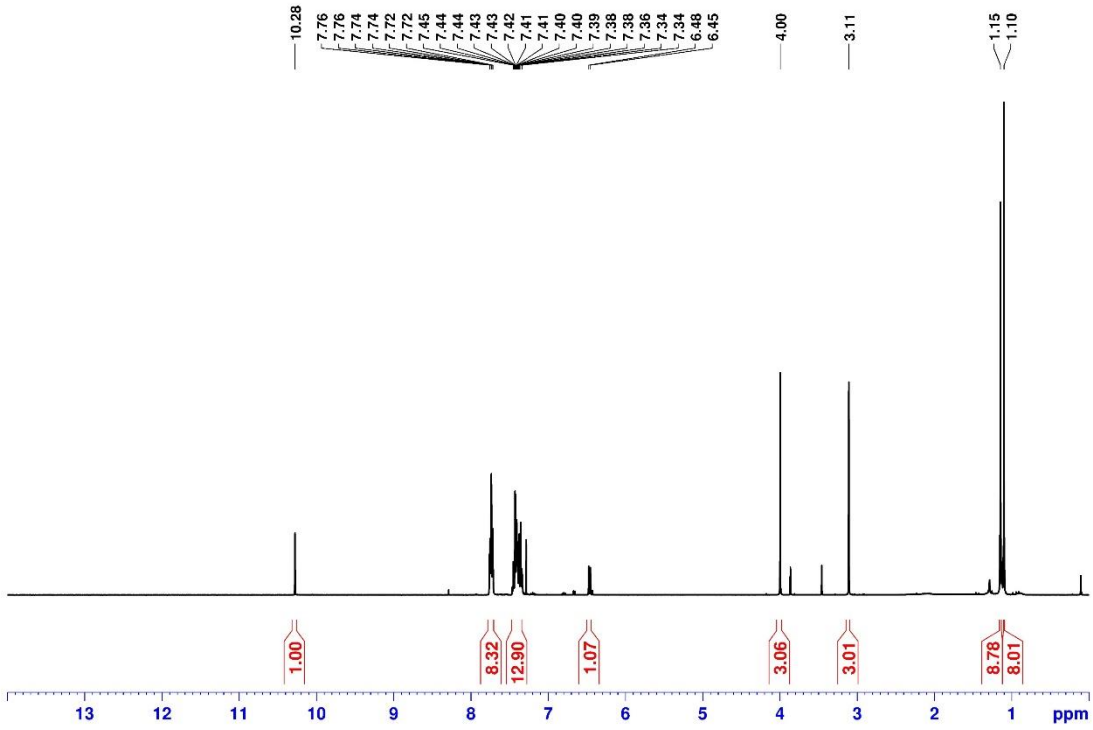
A. 66 ^{1}H NMR spectrum of **(4.05)**



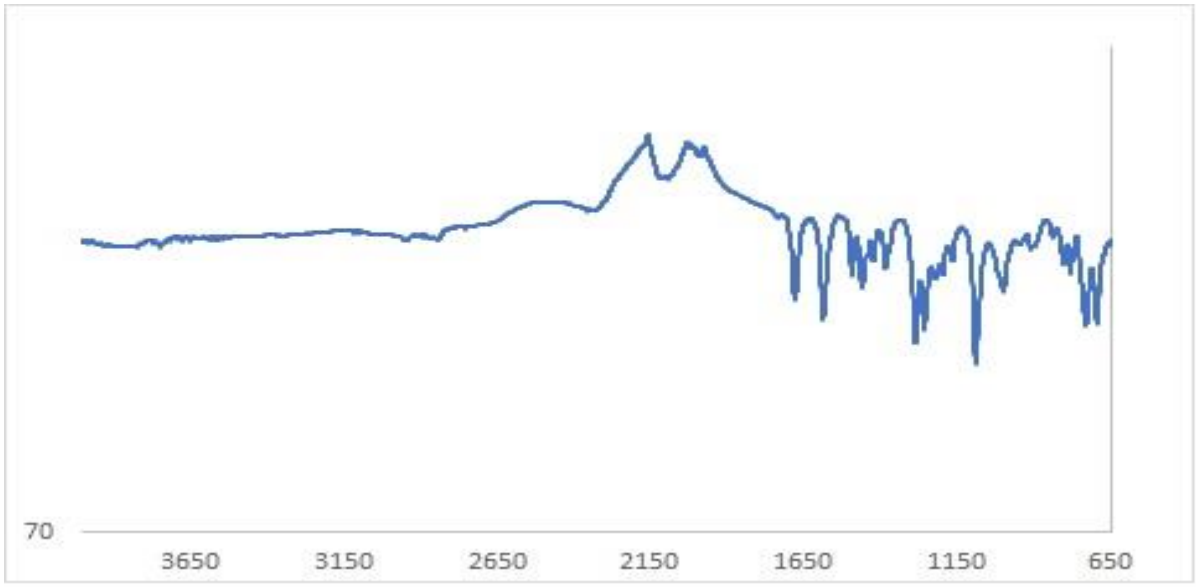
A. 67 ^{13}C NMR spectrum of **(4.05)**



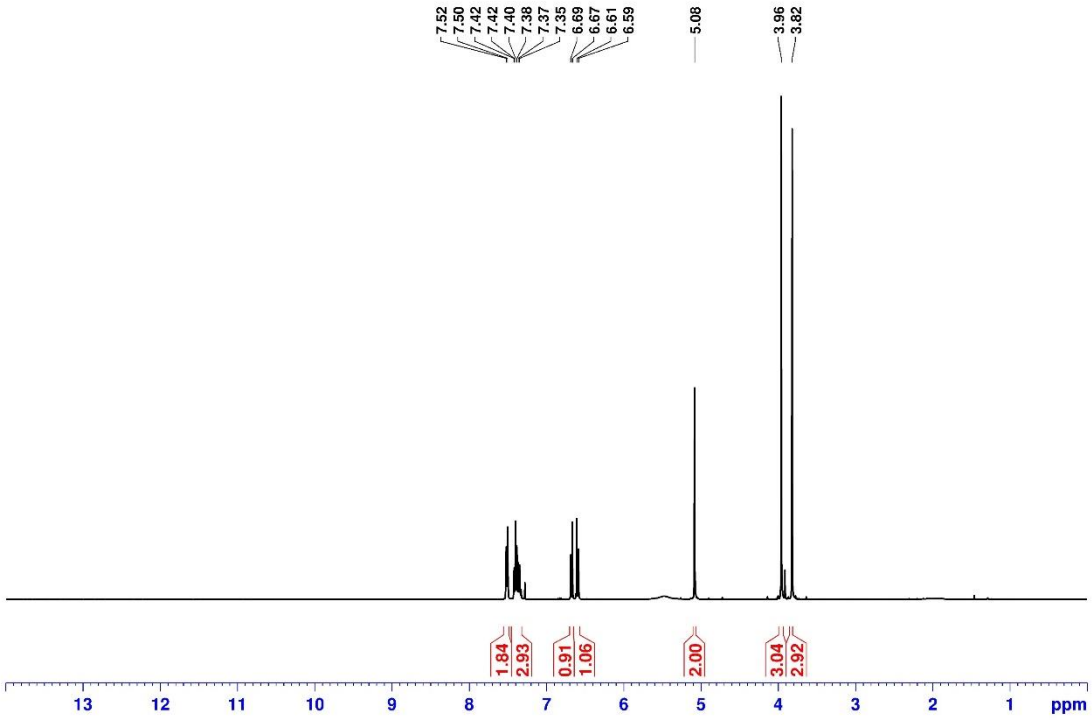
A. 68 ESI-MS of **(4.05)**, positive mode m/z 393 $[M+H]^+$



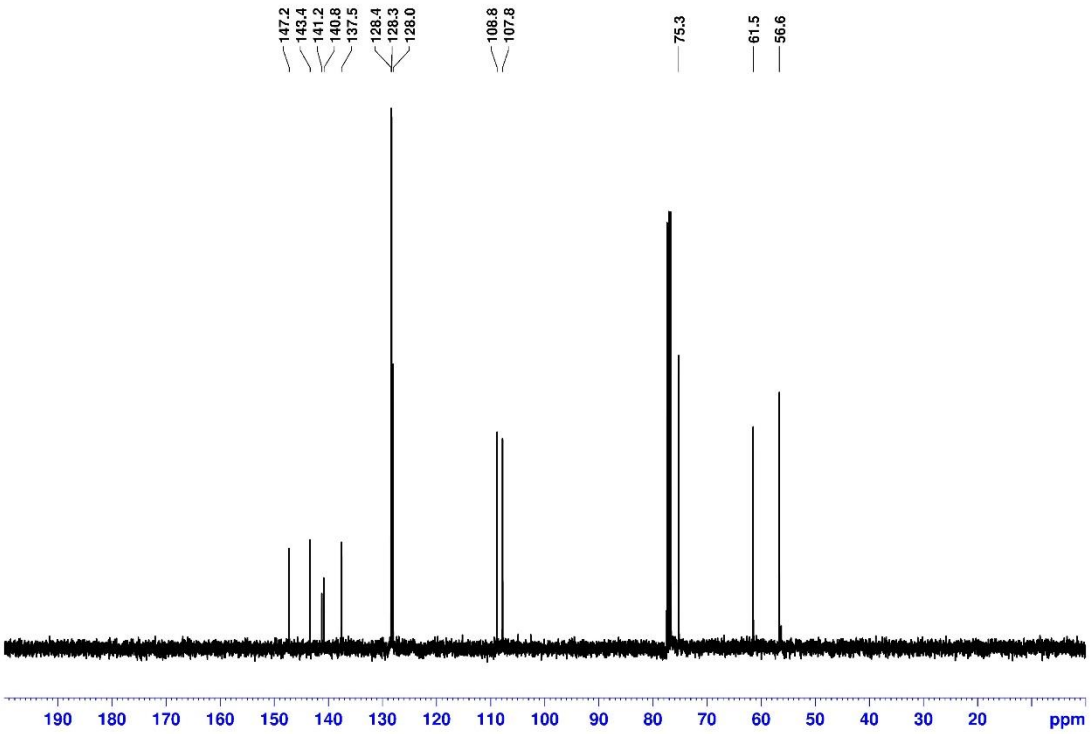
A. 69 ^{1}H NMR spectrum of **(4.06)**



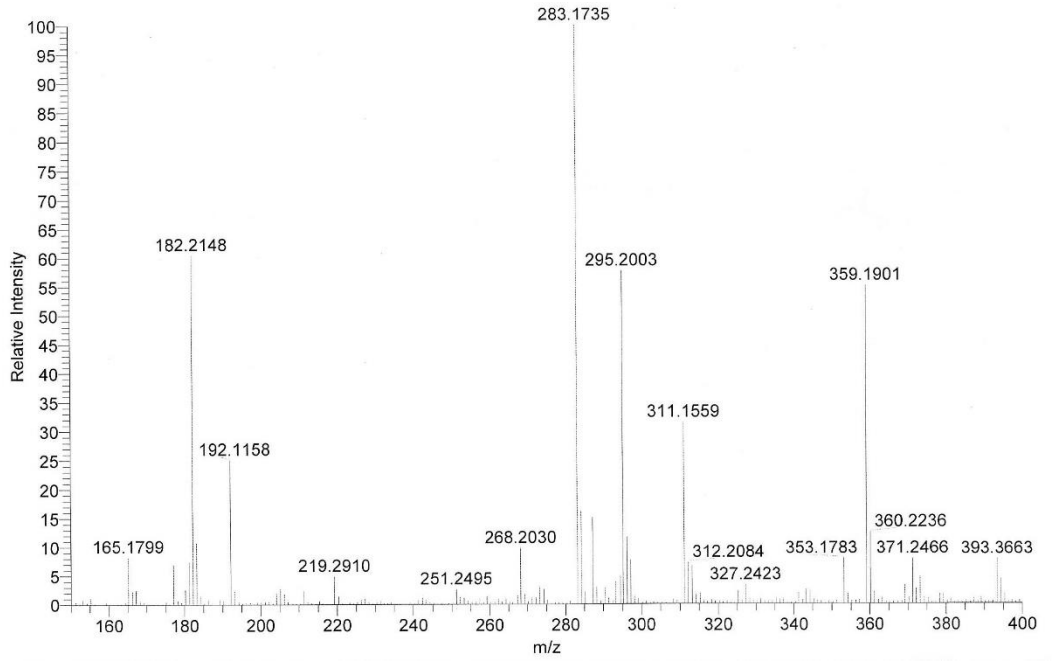
A. 70 IR spectrum of **(4.06)**



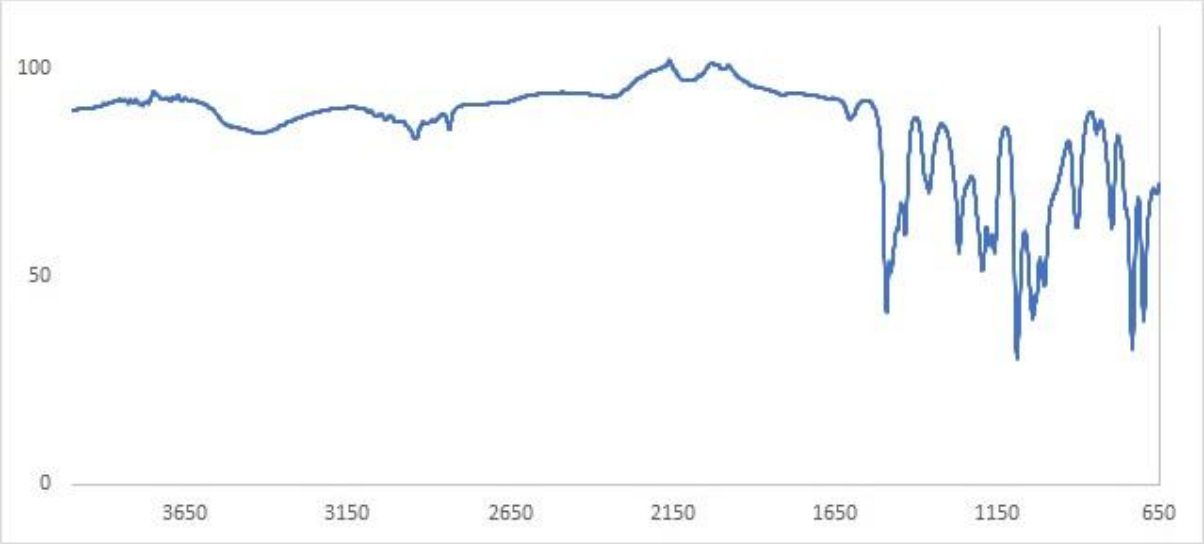
A. 71 ^{1}H NMR spectrum of **(4.08)**



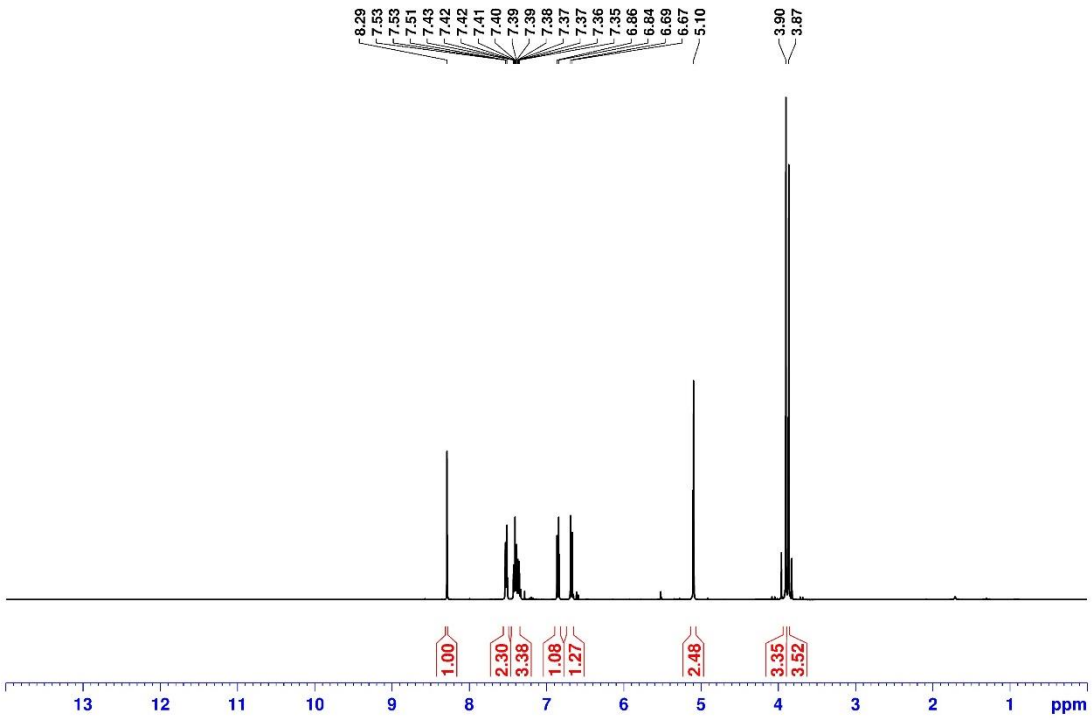
A. 72 ^{13}C NMR spectrum of **(4.08)**



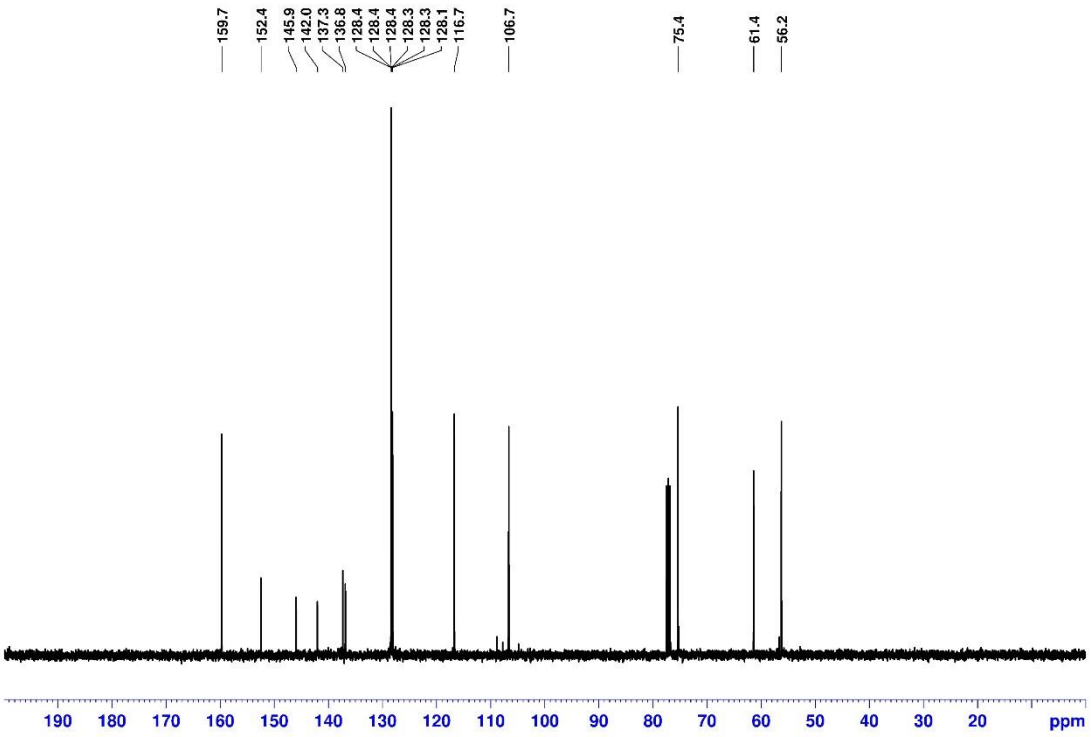
A. 73 ESI-MS of **(4.08)**, positive mode m/z 283 $[M+Na]^+$



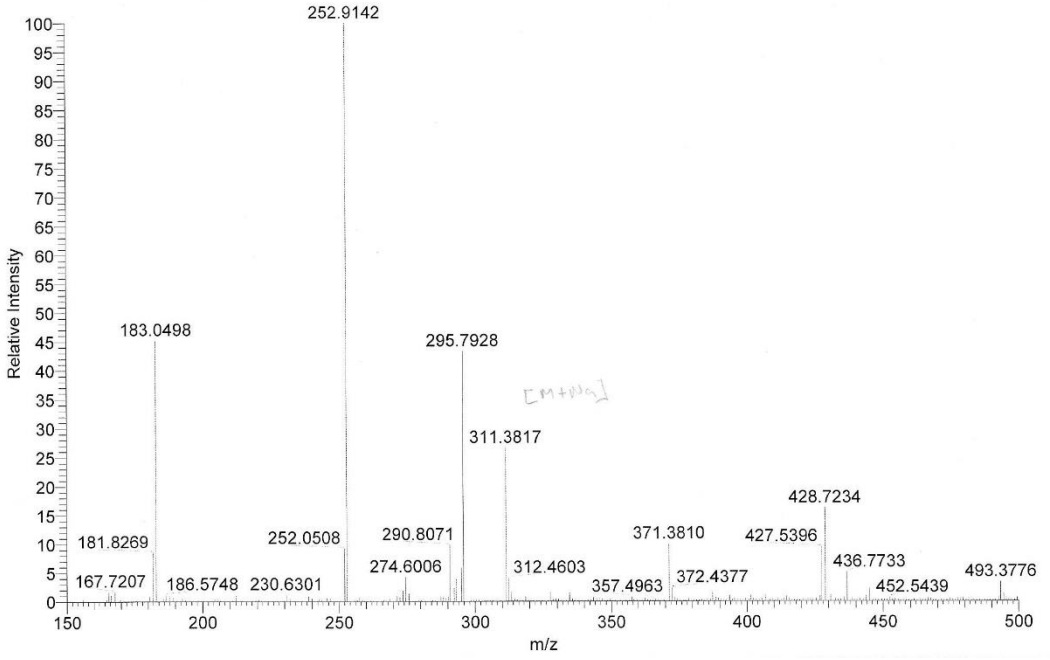
A. 74 IR spectrum of **(4.08)**



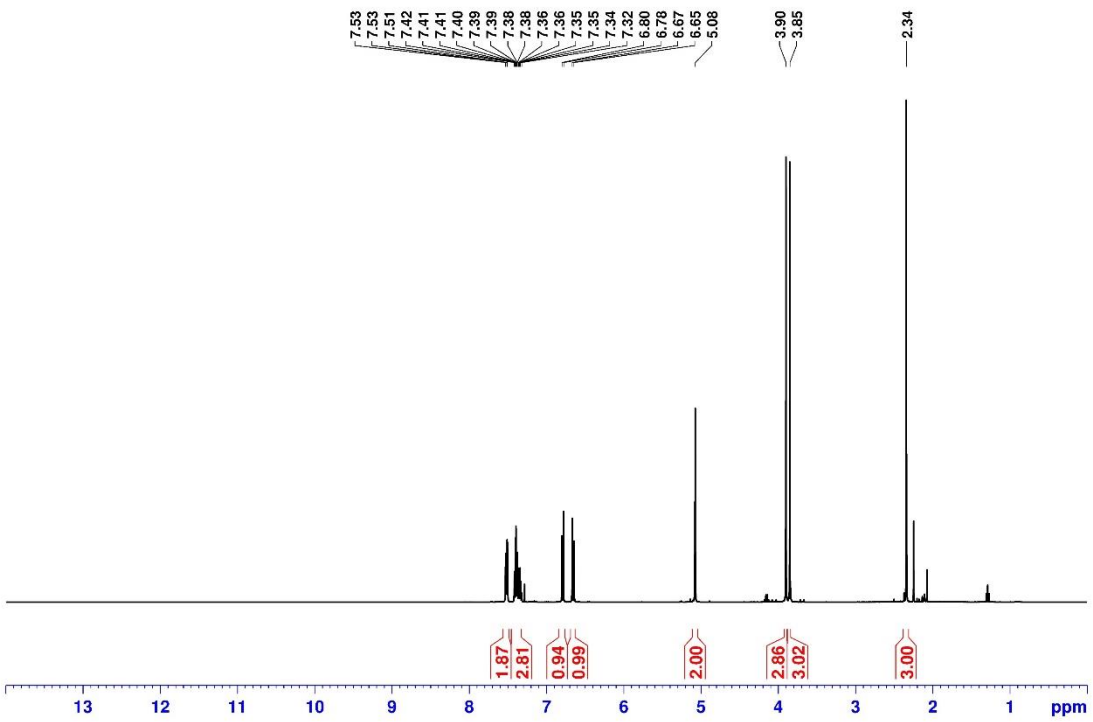
A. 75 ^{1}H NMR spectrum of **(4.10)**



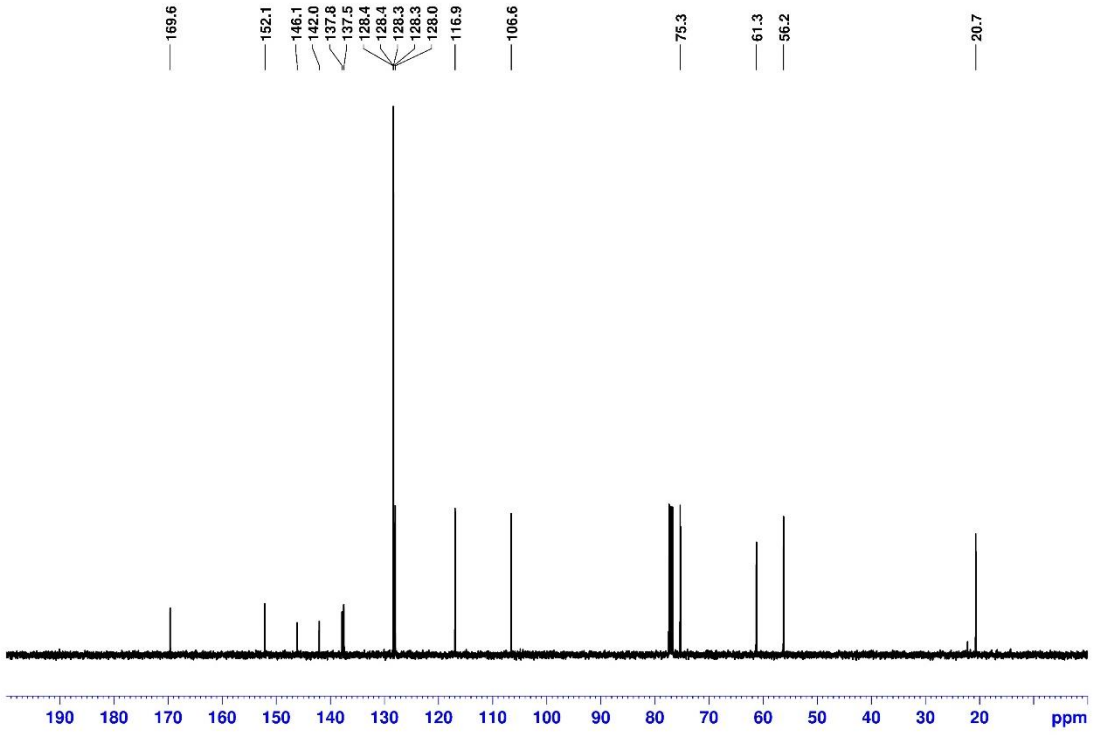
A. 76 ^{13}C NMR spectrum of **(4.10)**



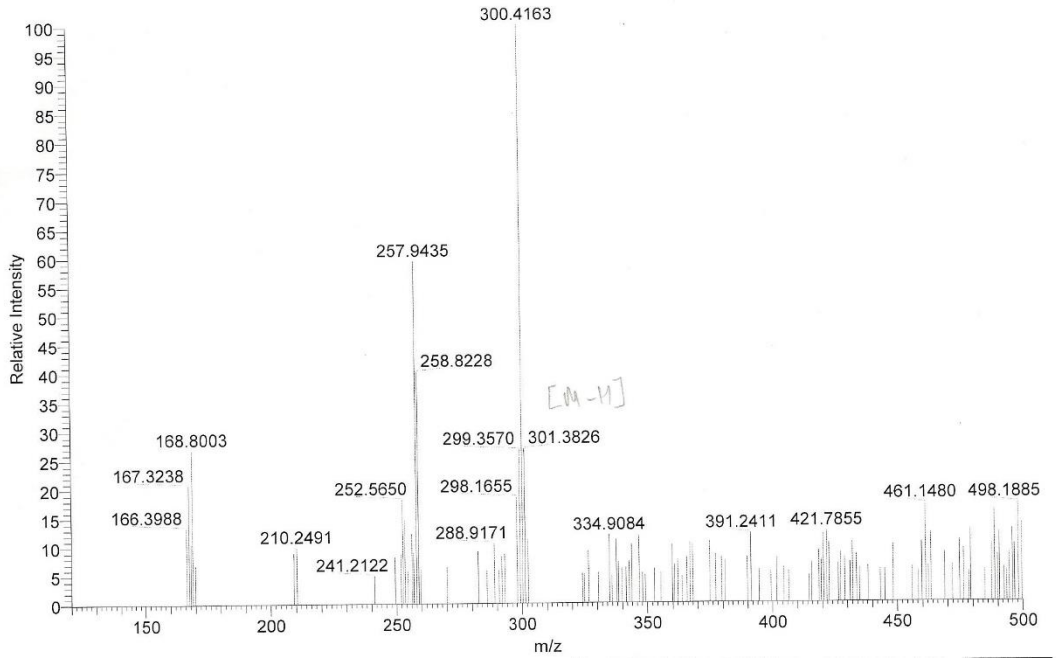
A. 77 ESI-MS of **(4.10)**, positive mode m/z 311 $[M+H]^+$



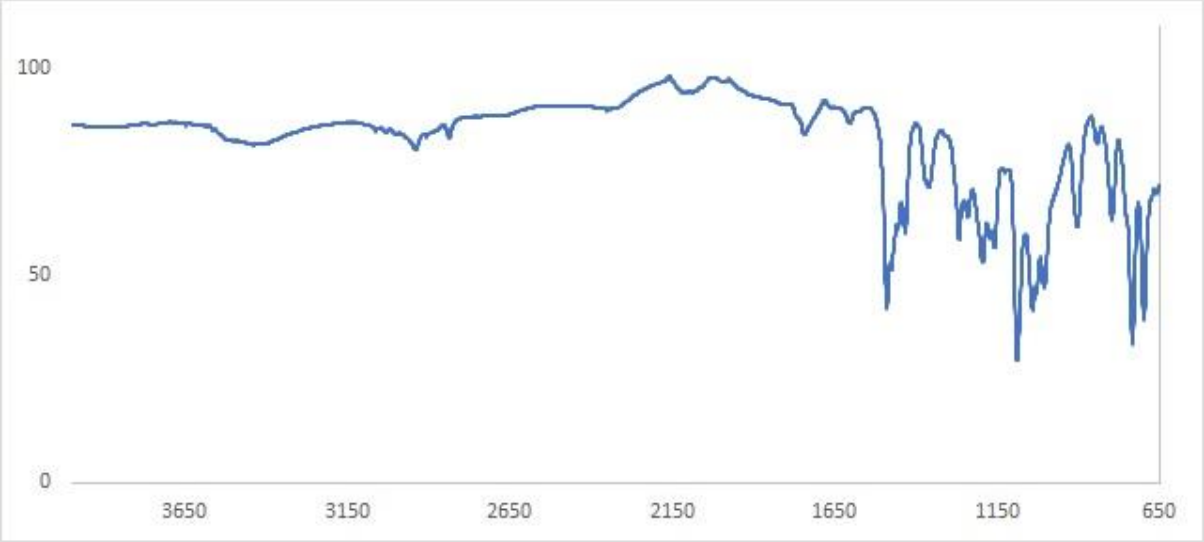
A. 78 ^{1}H NMR spectrum of **(4.11)**



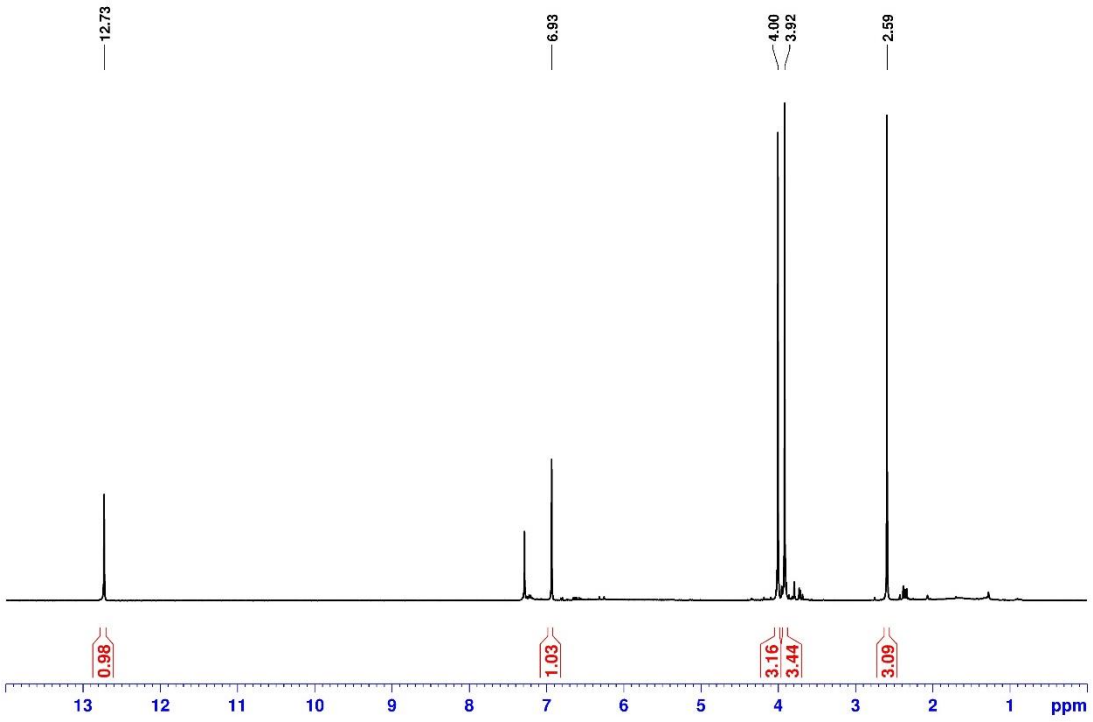
A. 79 ^{13}C NMR spectrum of **(4.11)**



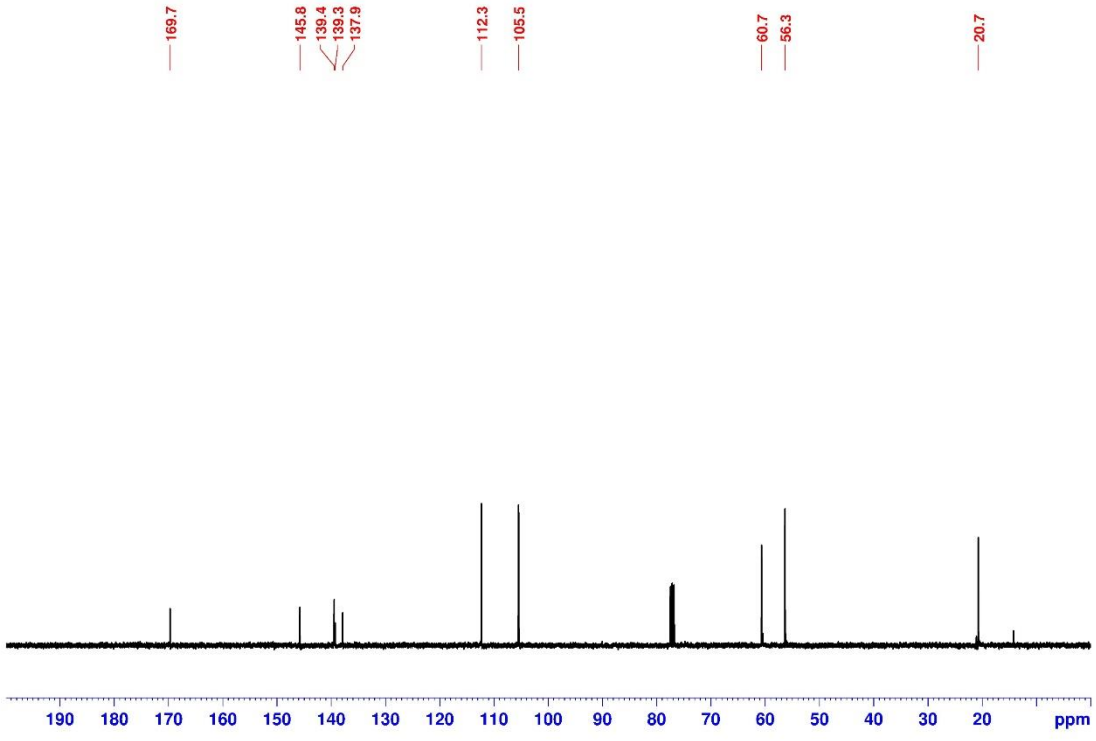
A. 80 ESI-MS of **(4.11)**, negative mode m/z 301 $[M+H]^-$



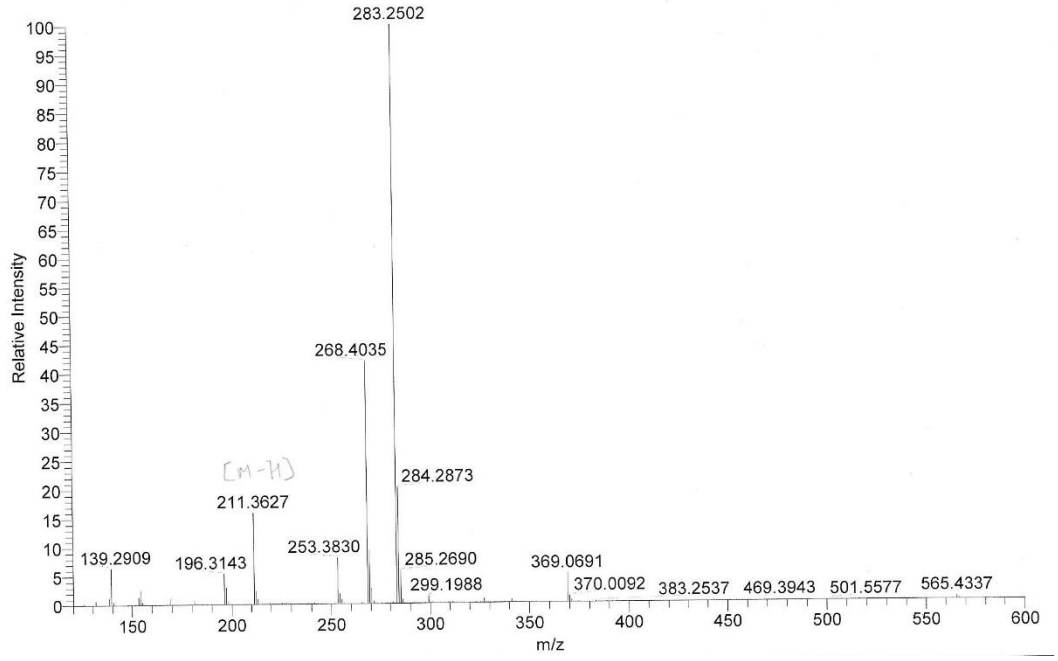
A. 81 IR spectrum of **(4.11)**



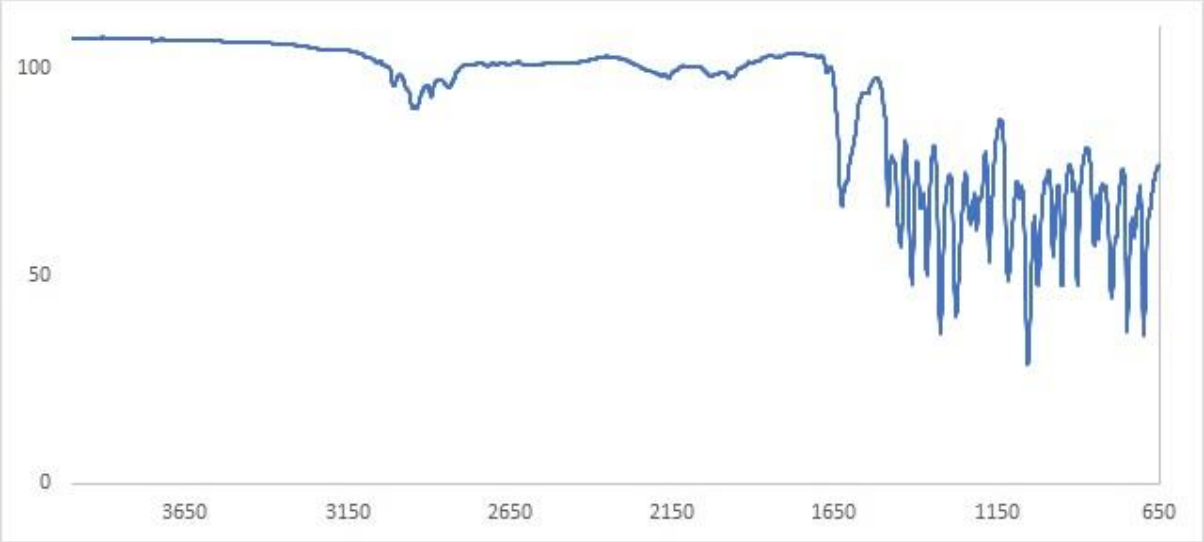
A. 82 ^{1}H NMR spectrum of **(4.13)**



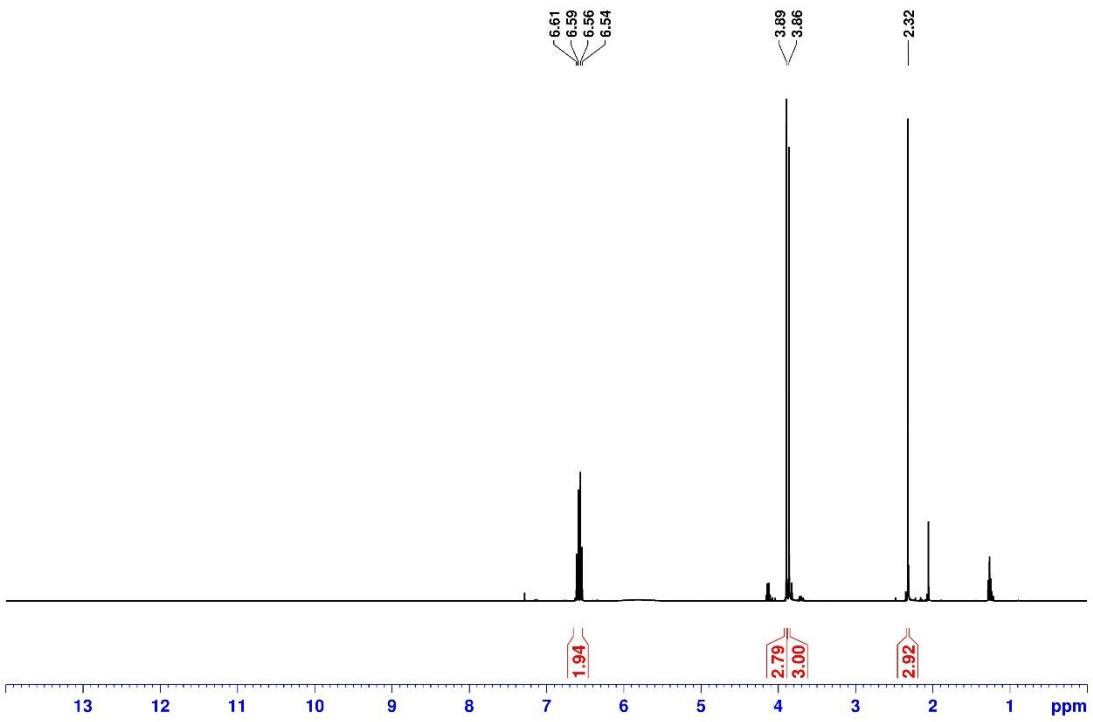
A. 83 ^{13}C NMR spectrum of **(4.13)**



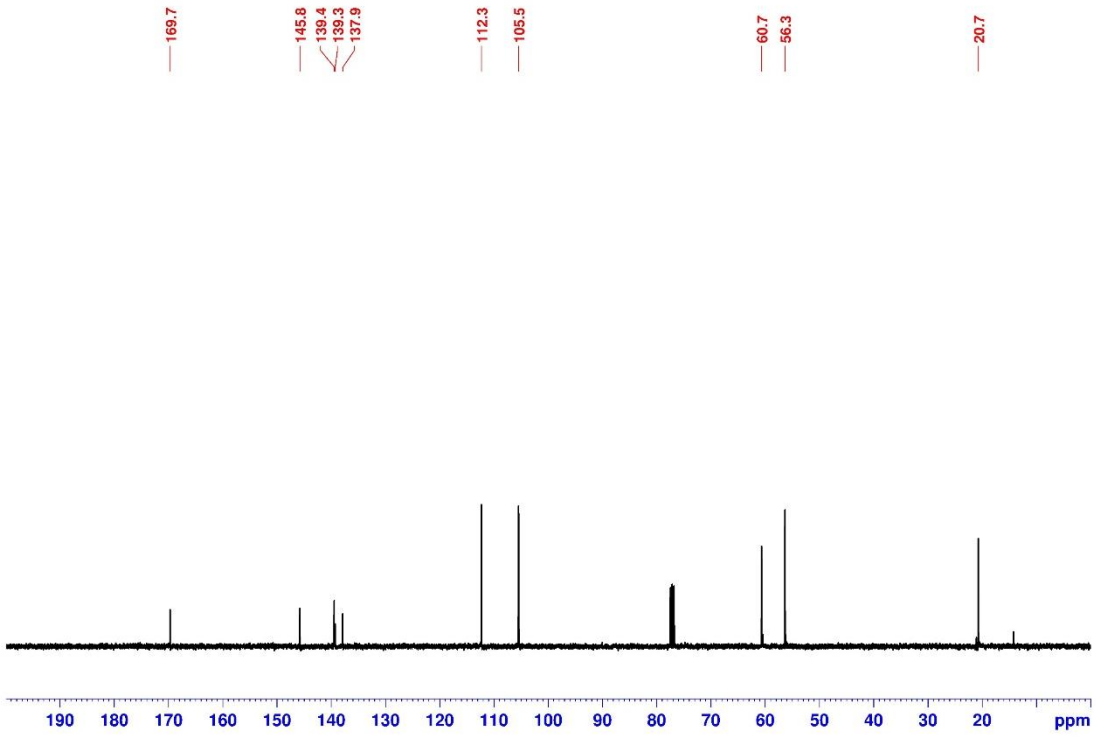
A. 84 ESI-MS of **(4.13)**, negative mode m/z 211 $[M+H]^-$



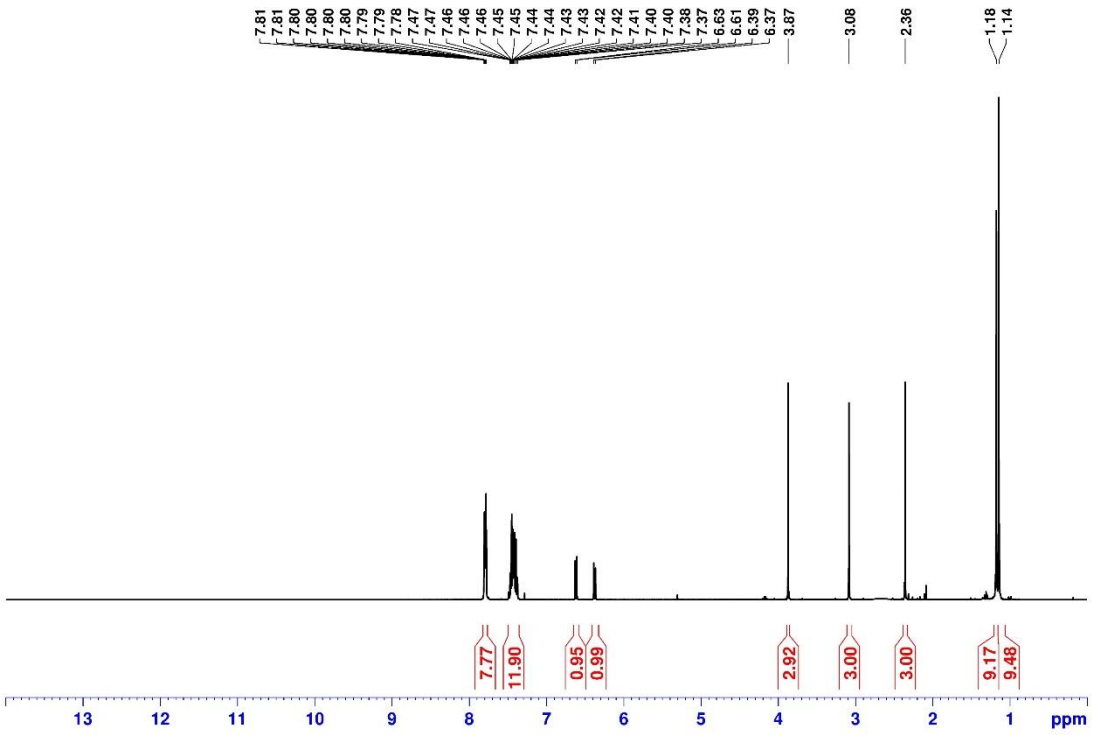
A. 85 IR spectrum of **(4.13)**



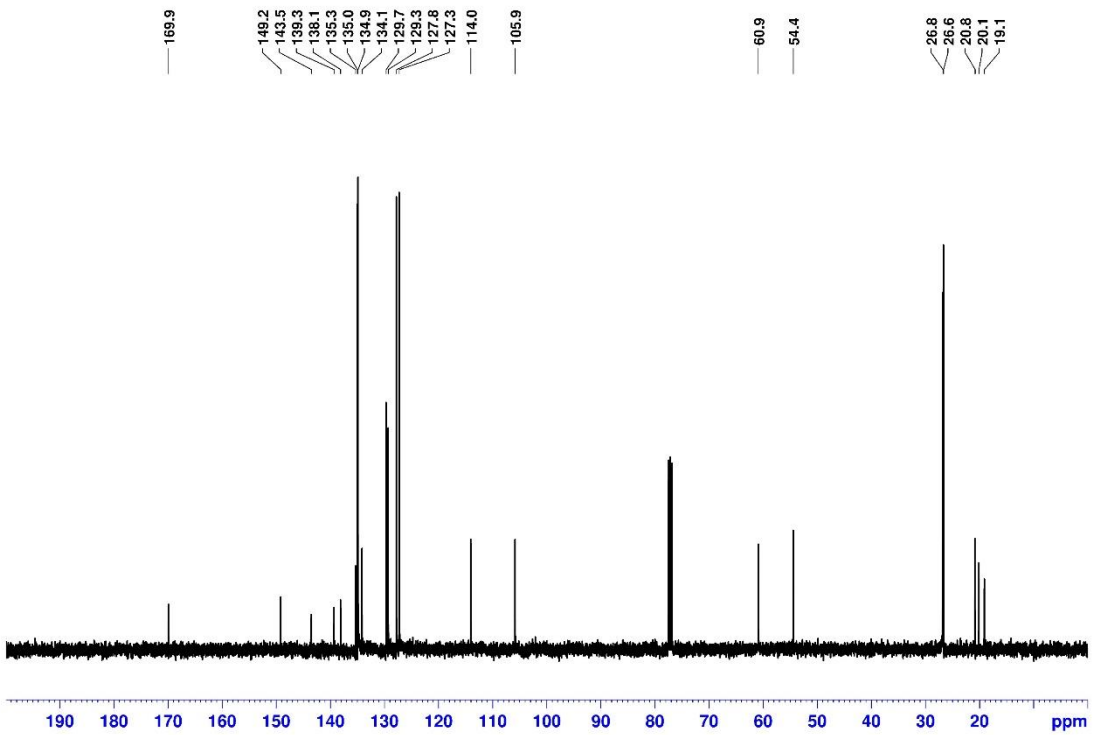
A. 86 ^{1}H NMR spectrum of **(4.14)**



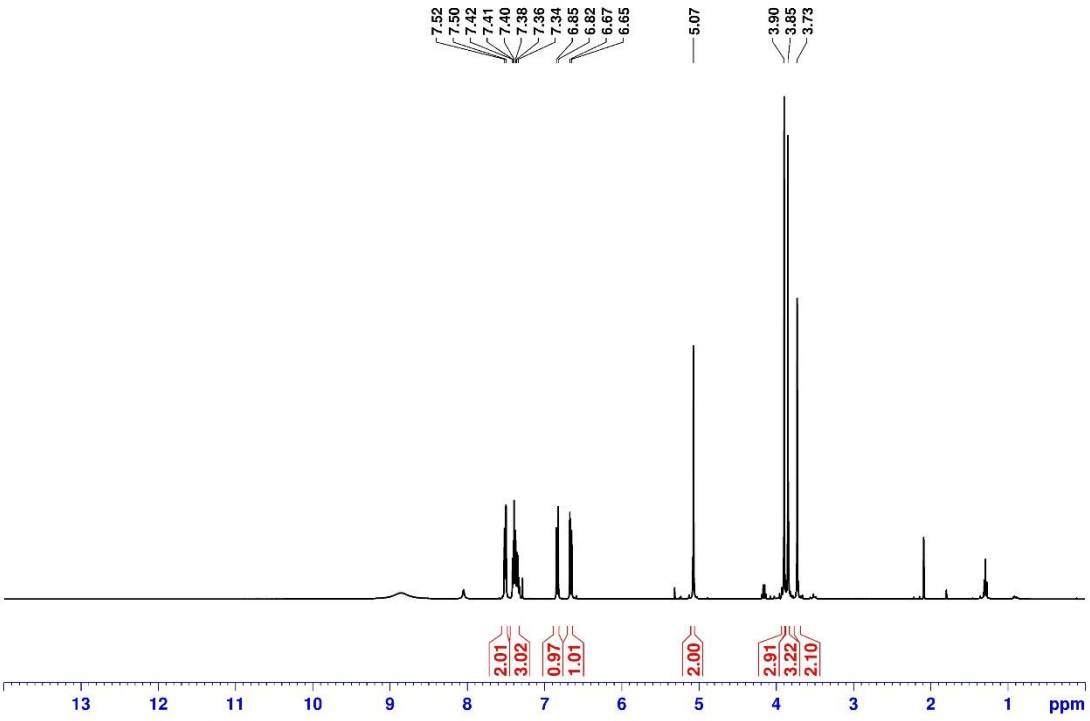
A. 87 ^{13}C NMR spectrum of **(4.14)**



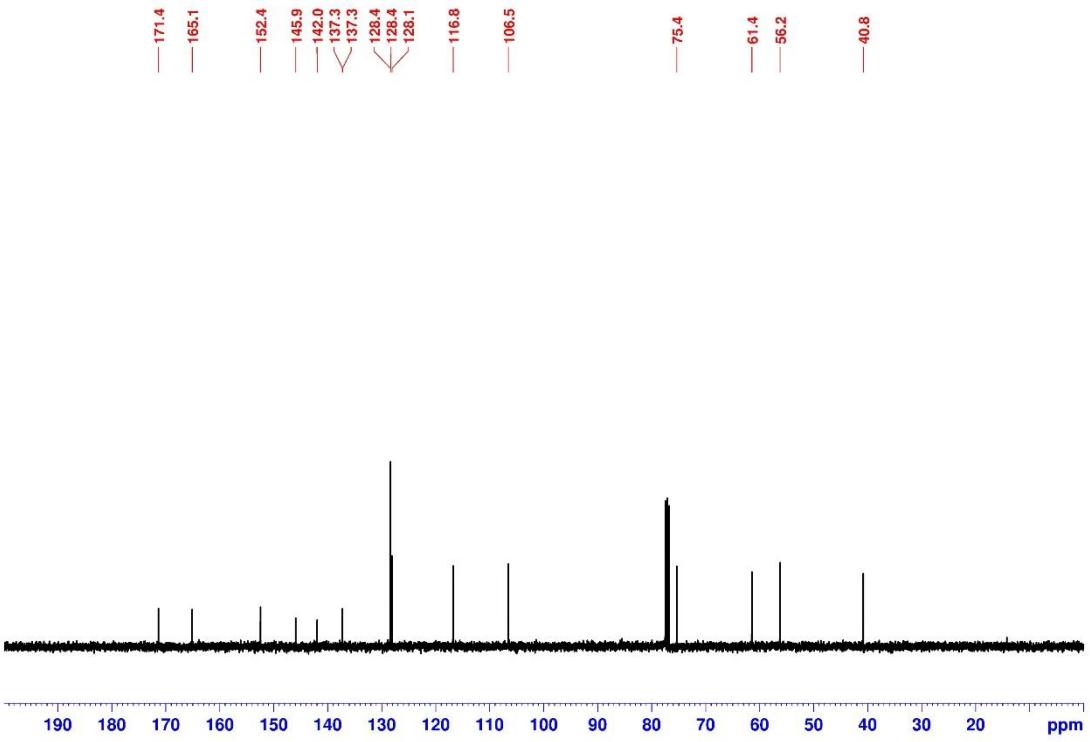
A. 88 ^{1}H NMR spectrum of **(4.15)**



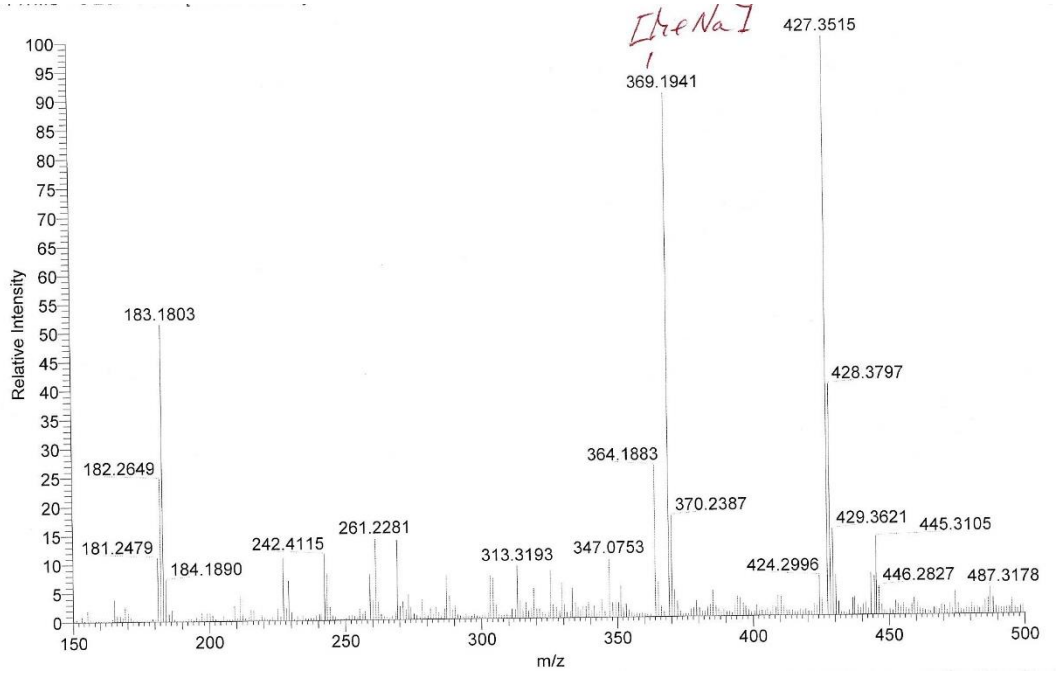
A. 89 ^{13}C NMR spectrum of **(4.15)**



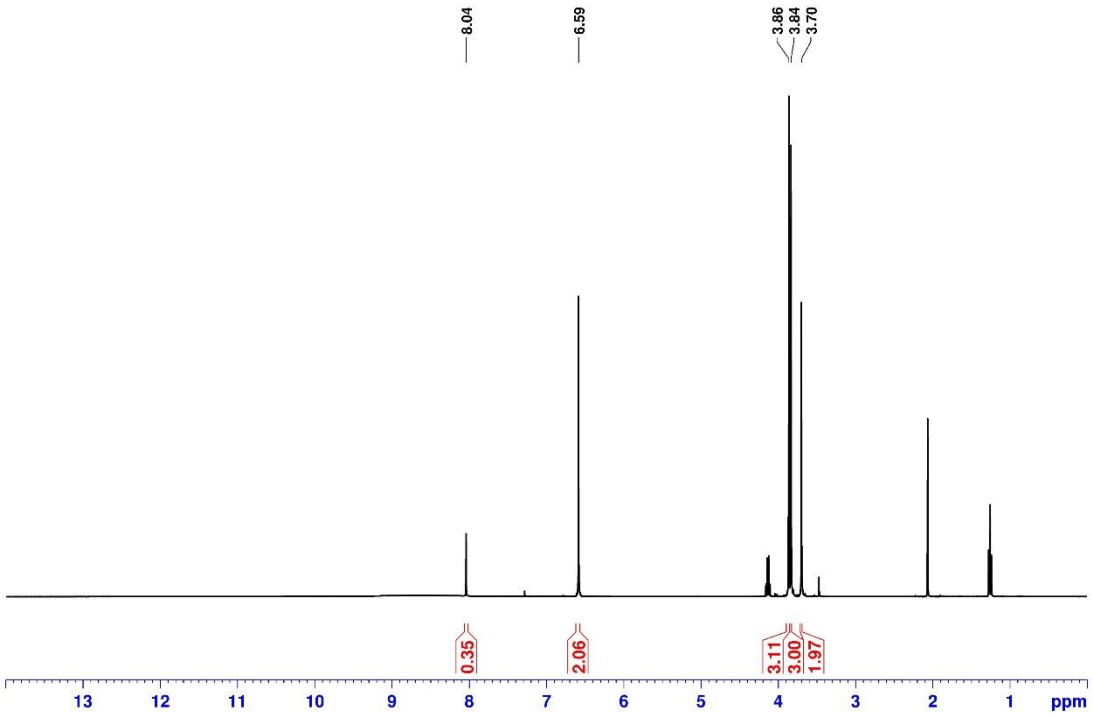
A. 90 ^{1}H NMR spectrum of **(4.18)**



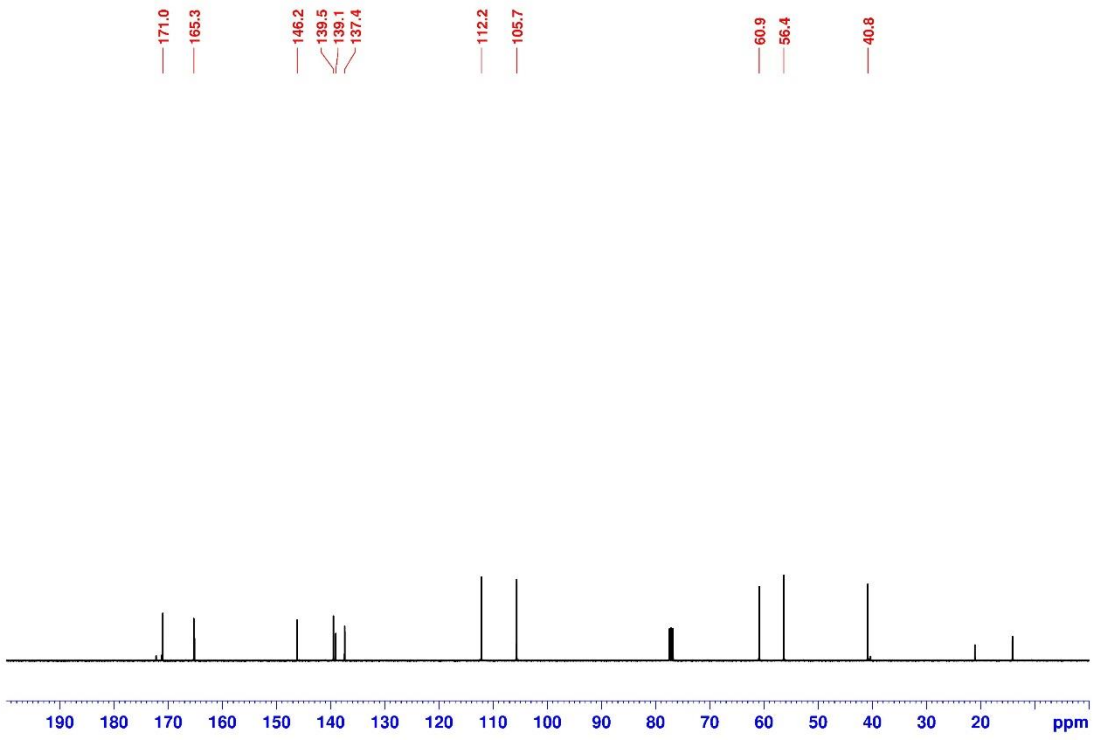
A. 91 ^{13}C NMR spectrum of **(4.18)**



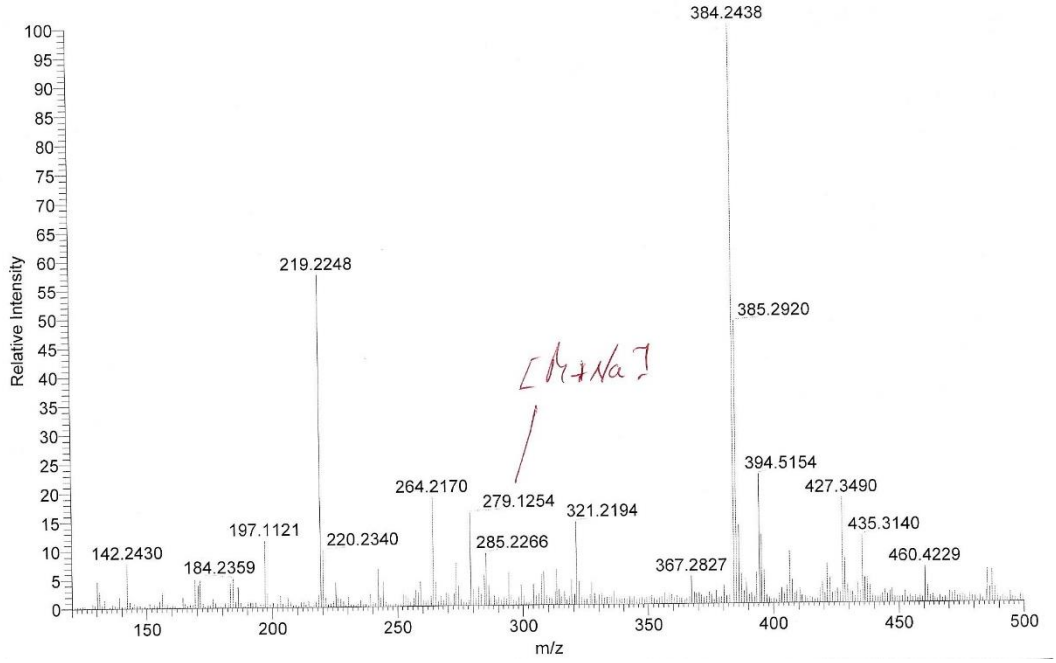
A. 92 ESI-MS of **(4.18)**, positive mode m/z 369 $[M+Na]^+$



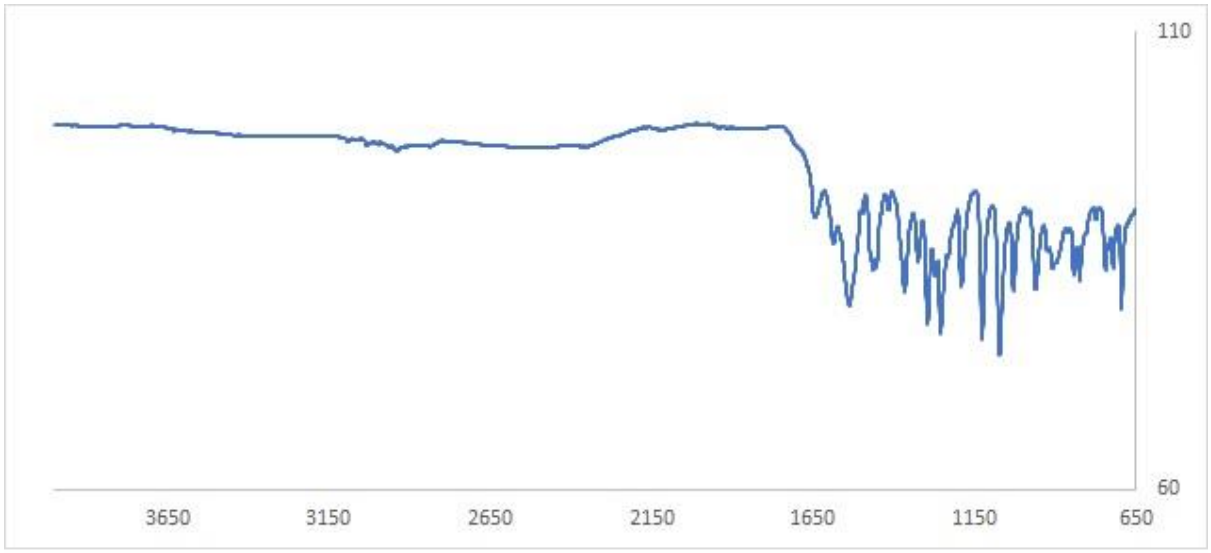
A. 93 ^{1}H NMR spectrum of **(4.22)**



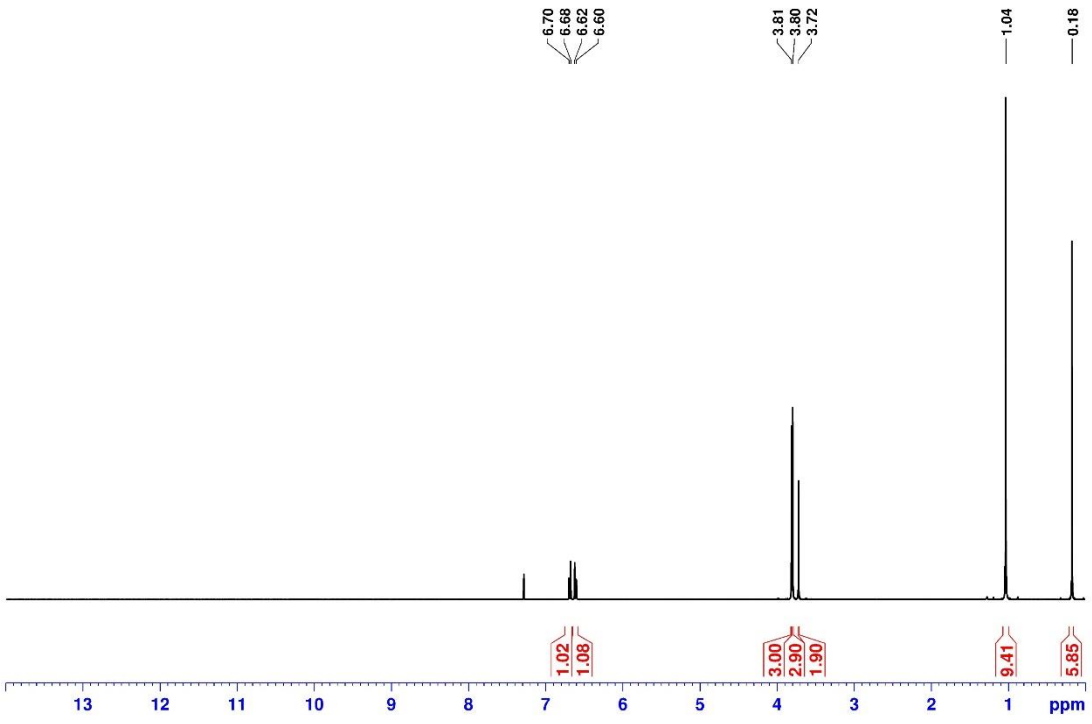
A. 94 ^{13}C NMR spectrum of **(4.22)**



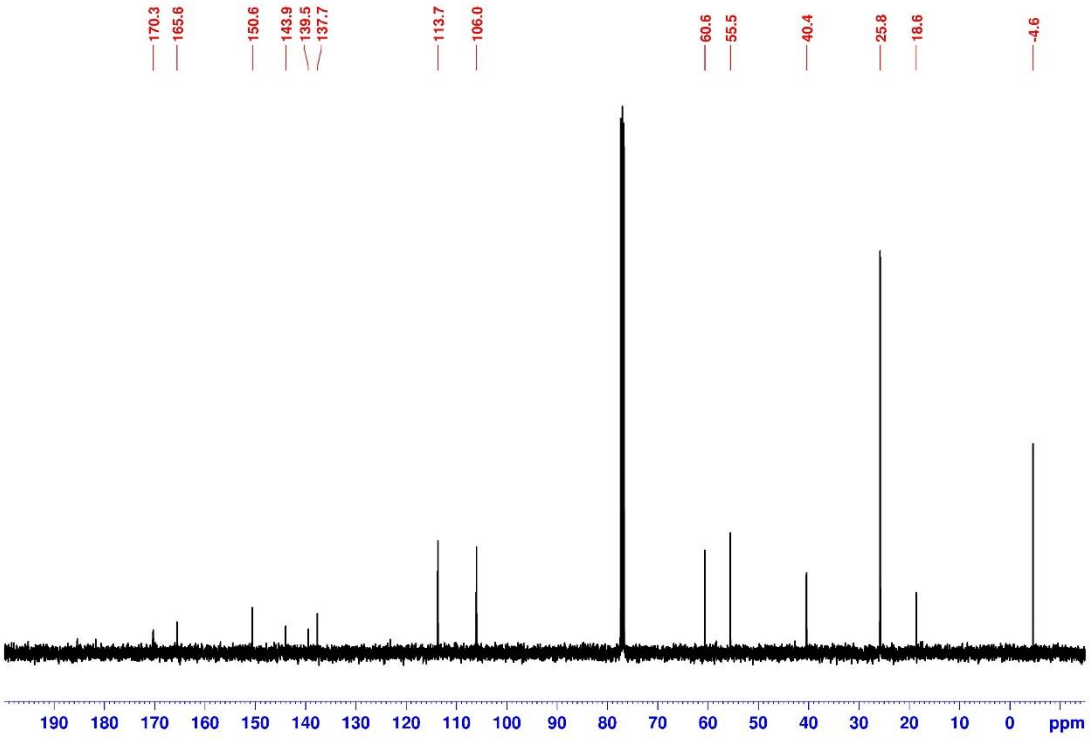
A. 95 ESI-MS of **(4.22)**, positive mode m/z 279 $[M+Na]^+$



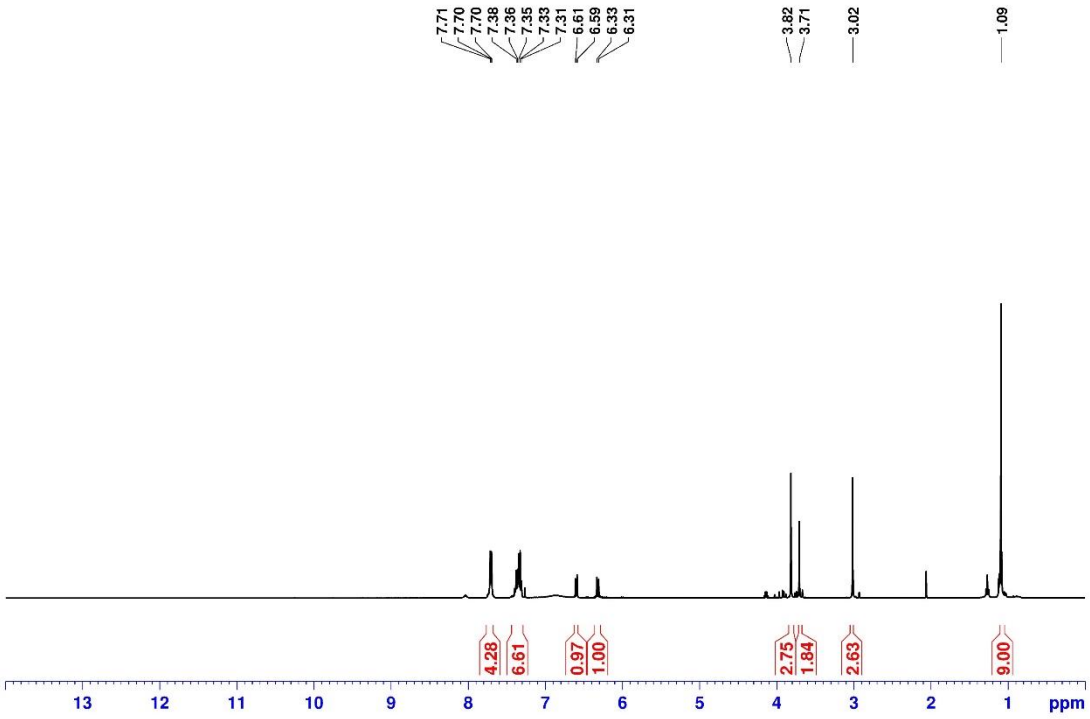
A. 96 IR spectrum of **(4.22)**



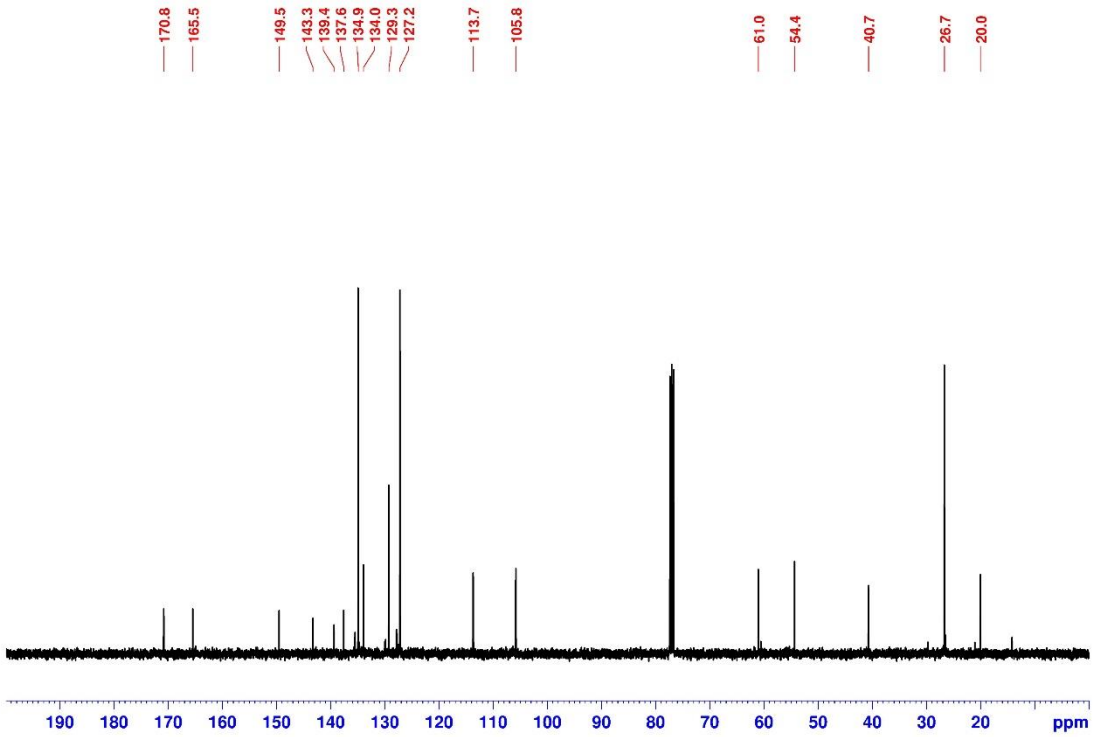
A. 97 ^{1}H NMR spectrum of **(4.23)**



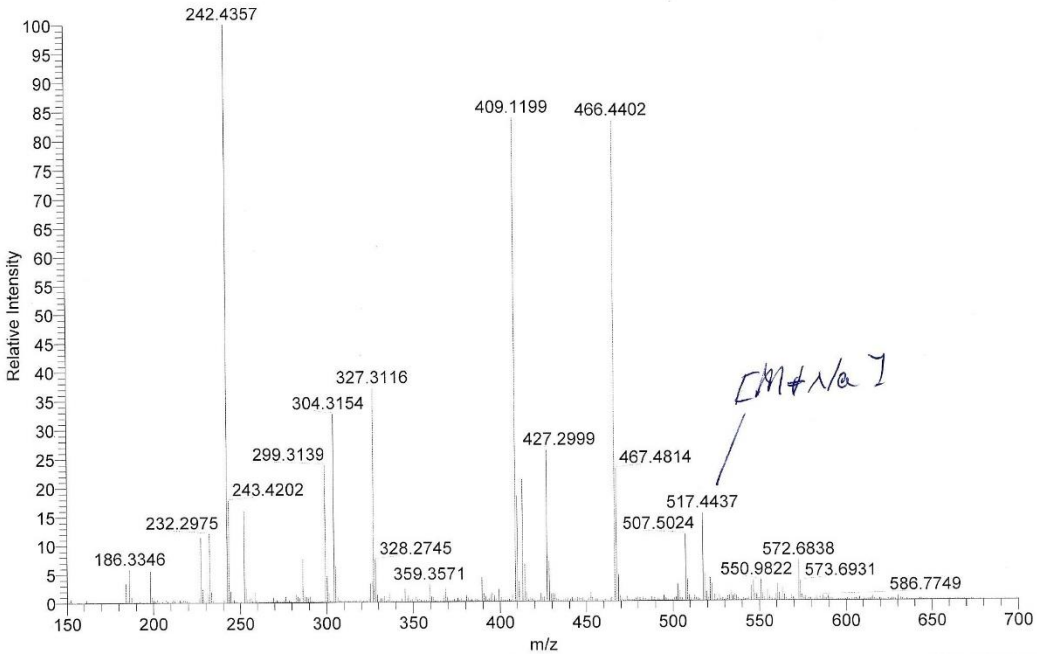
A. 98 ^{13}C NMR spectrum of **(4.23)**



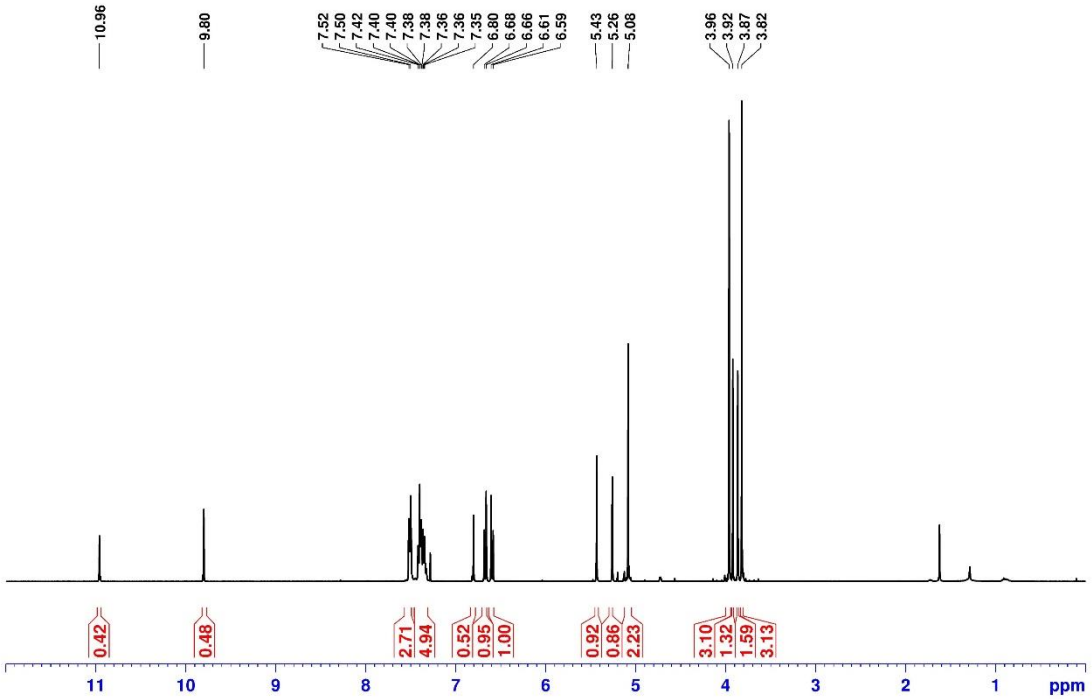
A. 99 ^{1}H NMR spectrum of **(4.25)**



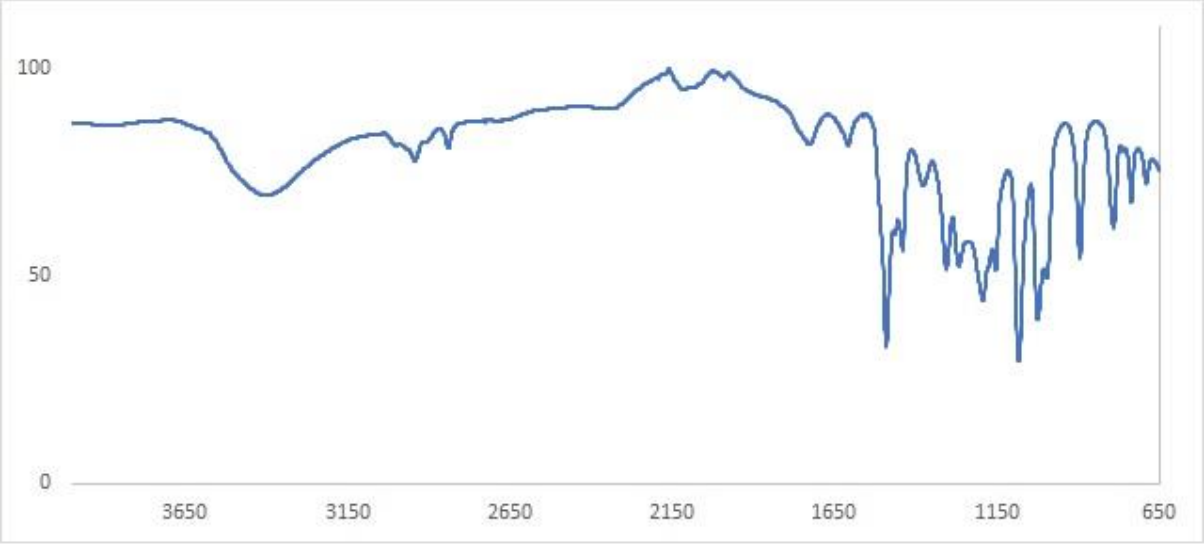
A. 100 ^{13}C NMR spectrum of **(4.25)**



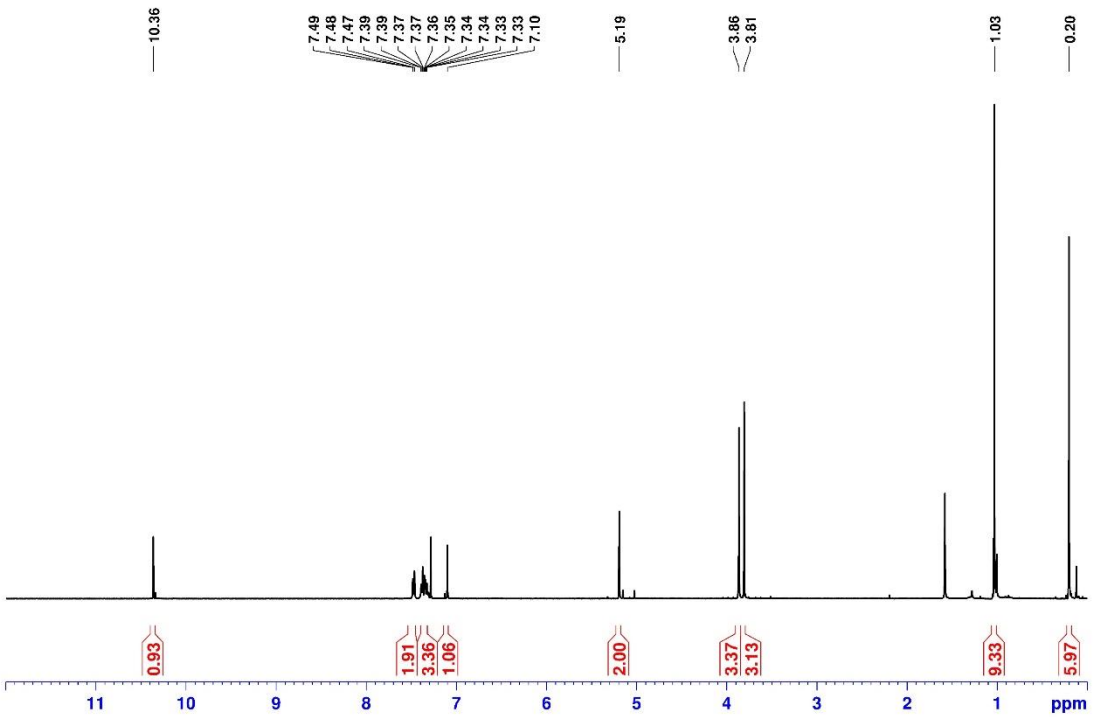
A. 101 ESI-MS of **(4.25)**, positive mode m/z 517 $[M+Na]^+$



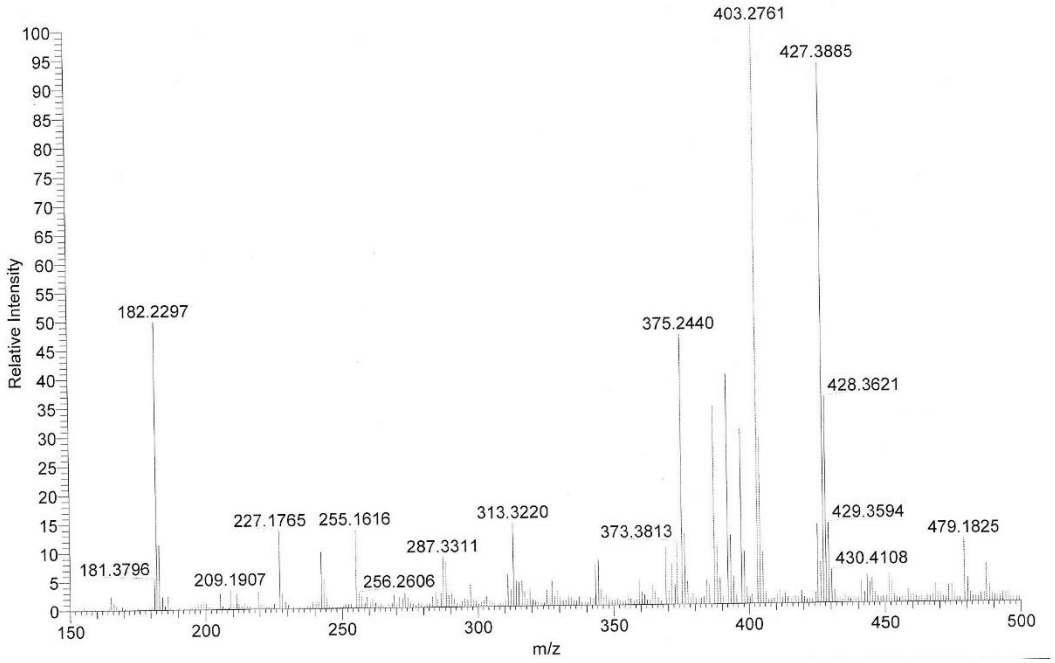
A. 102 ^{1}H NMR spectrum of **(4.27)**



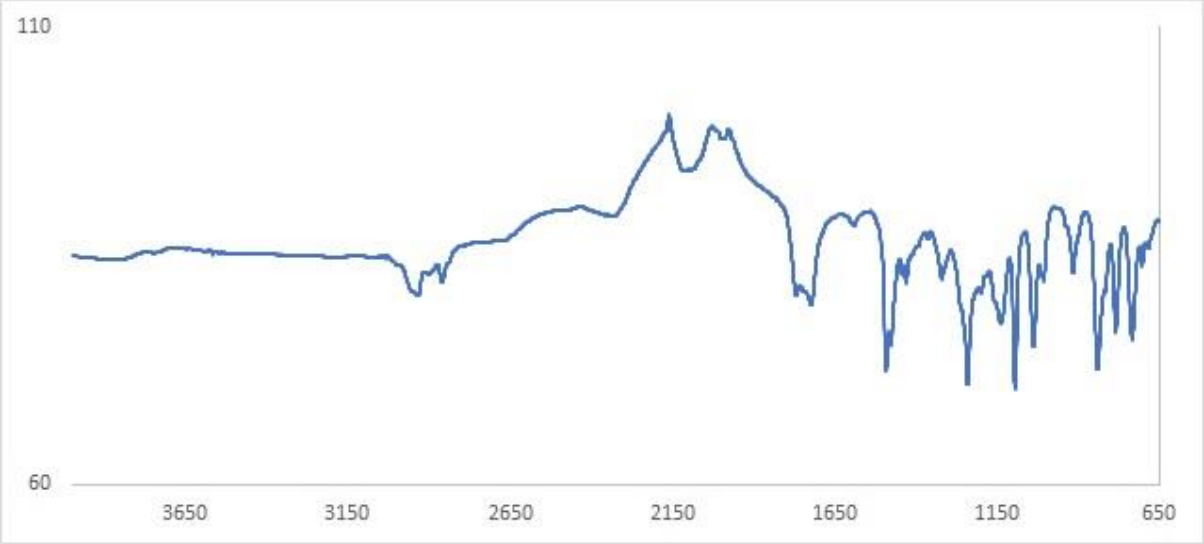
A. 103 IR spectrum of **(4.27)**



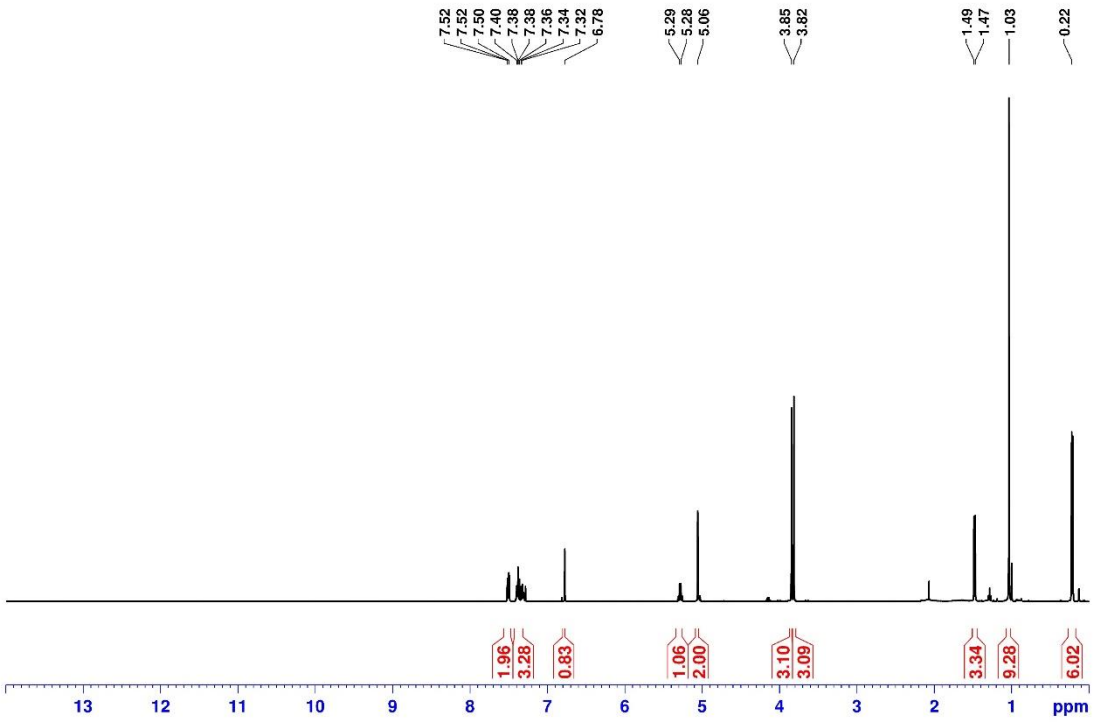
A. 104 ^{1}H NMR spectrum of **(4.28)**



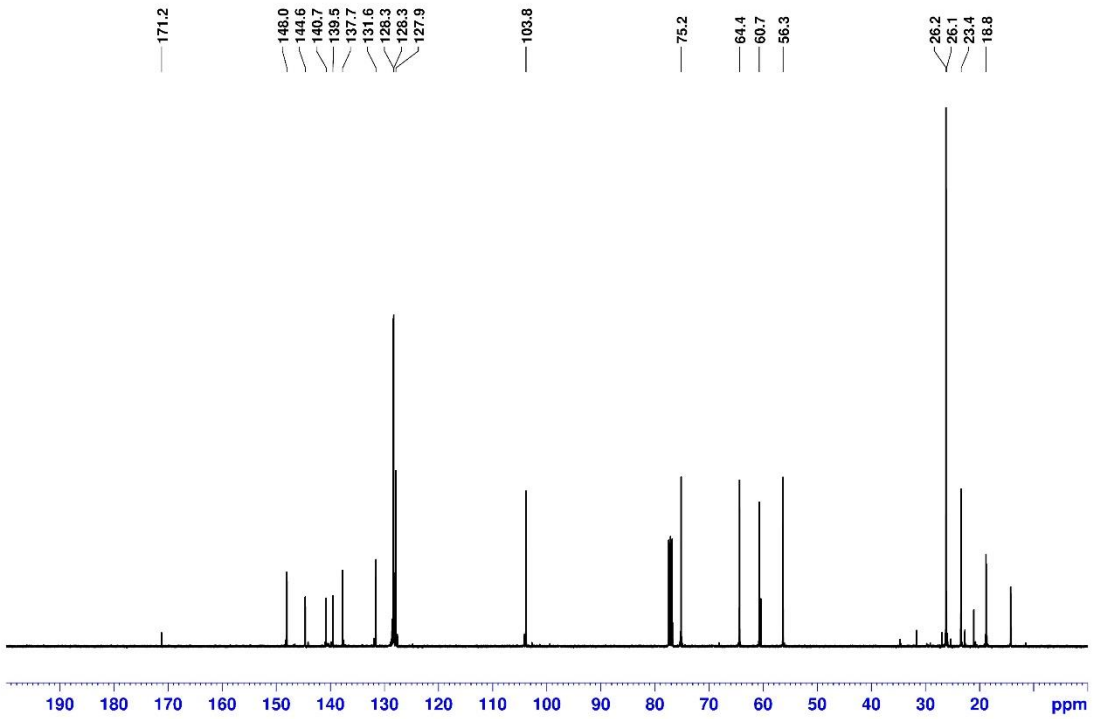
A. 105 ESI-MS of **(4.28)**, positive mode m/z 403 $[M+H]^{+}$



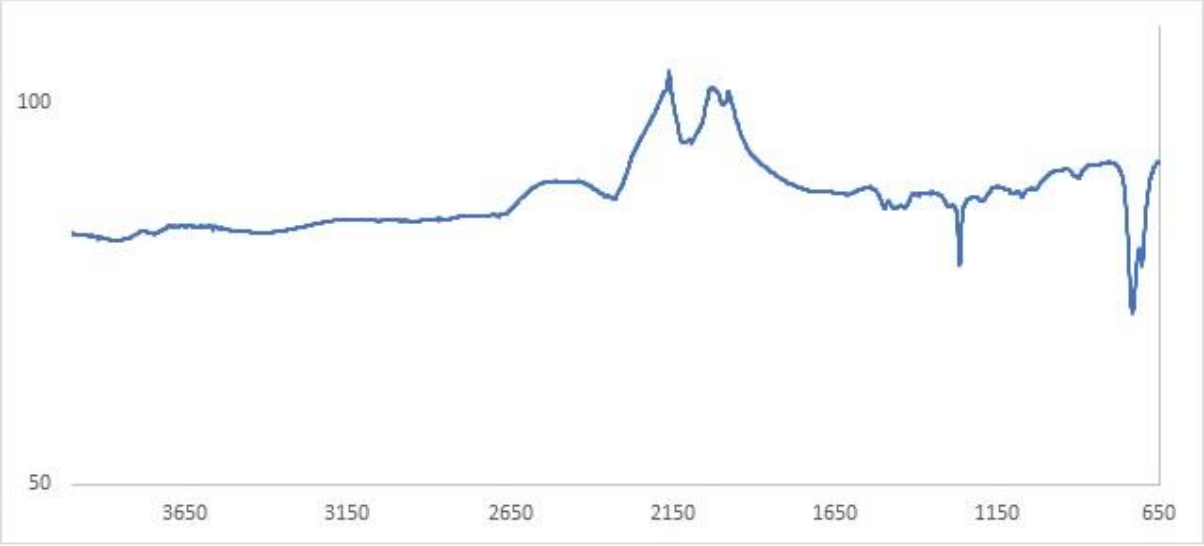
A. 106 IR spectrum of **(4.28)**



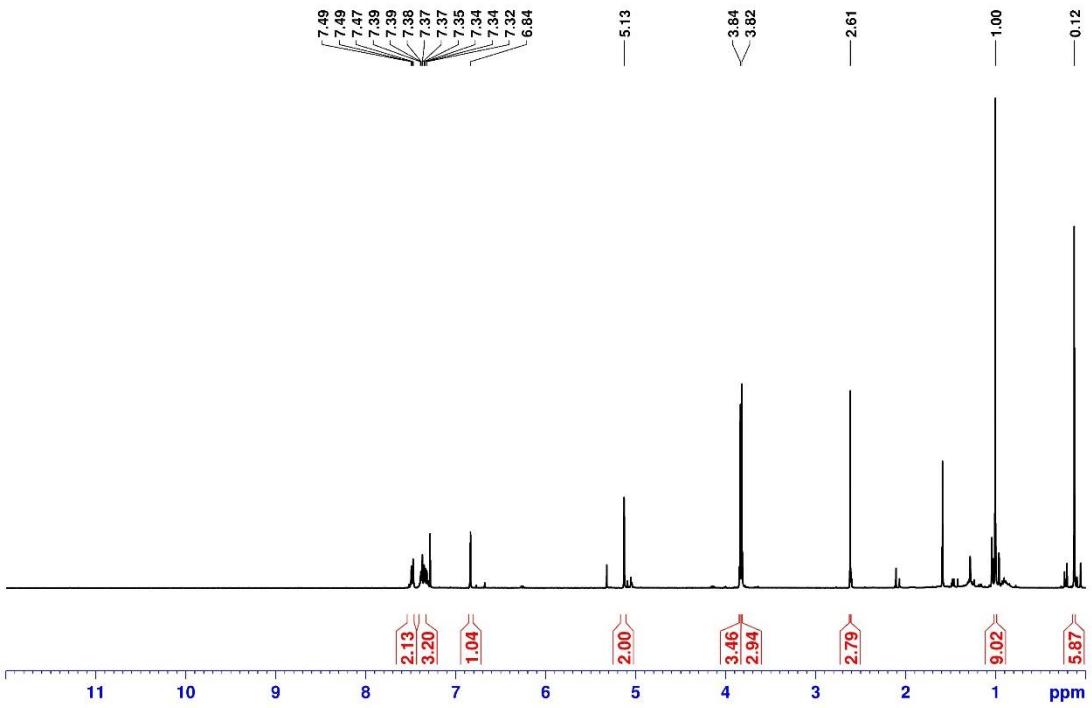
A. 107 ^{1}H NMR spectrum of **(4.30)**



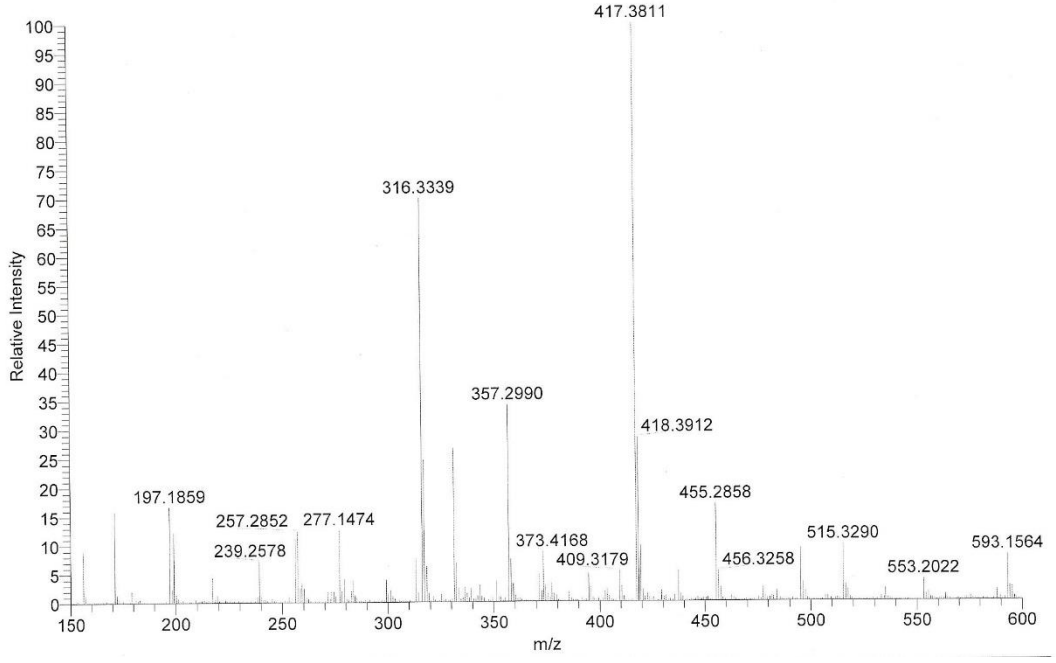
A. 108 ^{13}C NMR spectrum of **(4.30)**



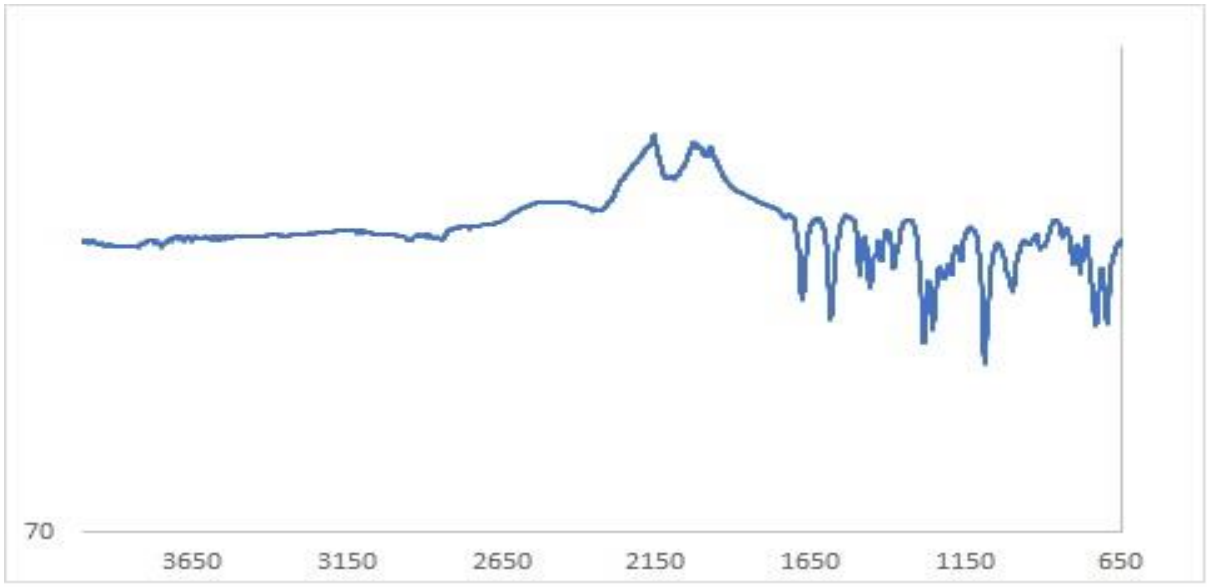
A. 109 IR spectrum of **(4.30)**



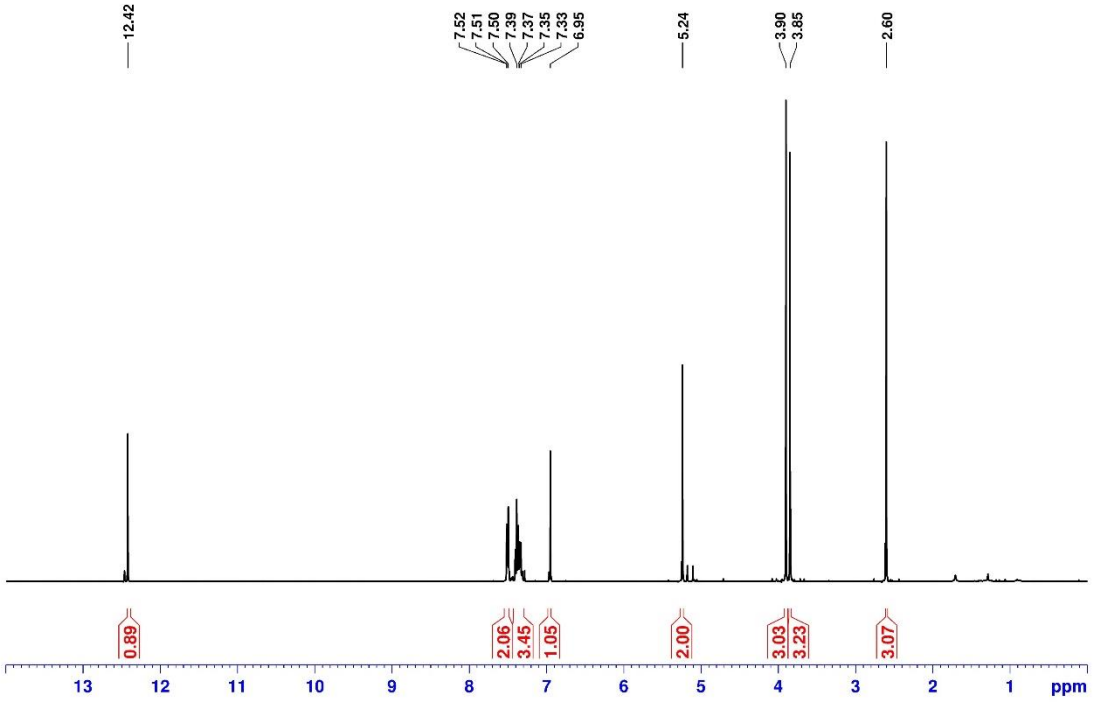
A. 110 ^{1}H NMR spectrum of **(4.31)**



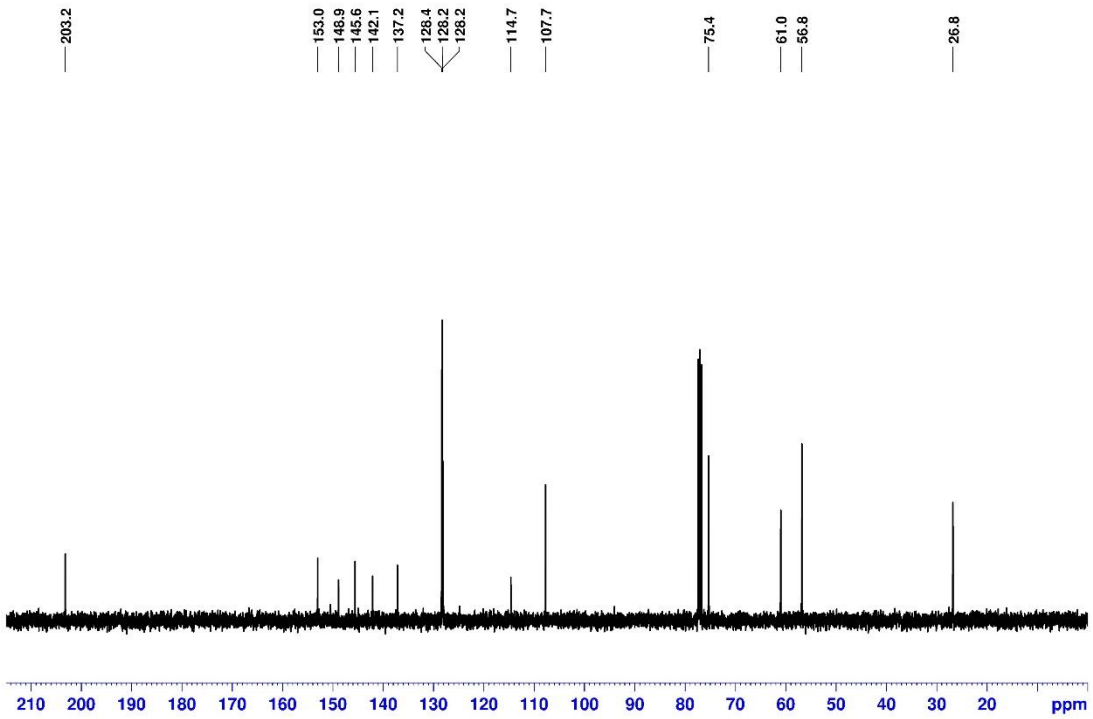
A. 111 ESI-MS of **(4.31)**, positive mode m/z 417 $[M+H]^{+}$



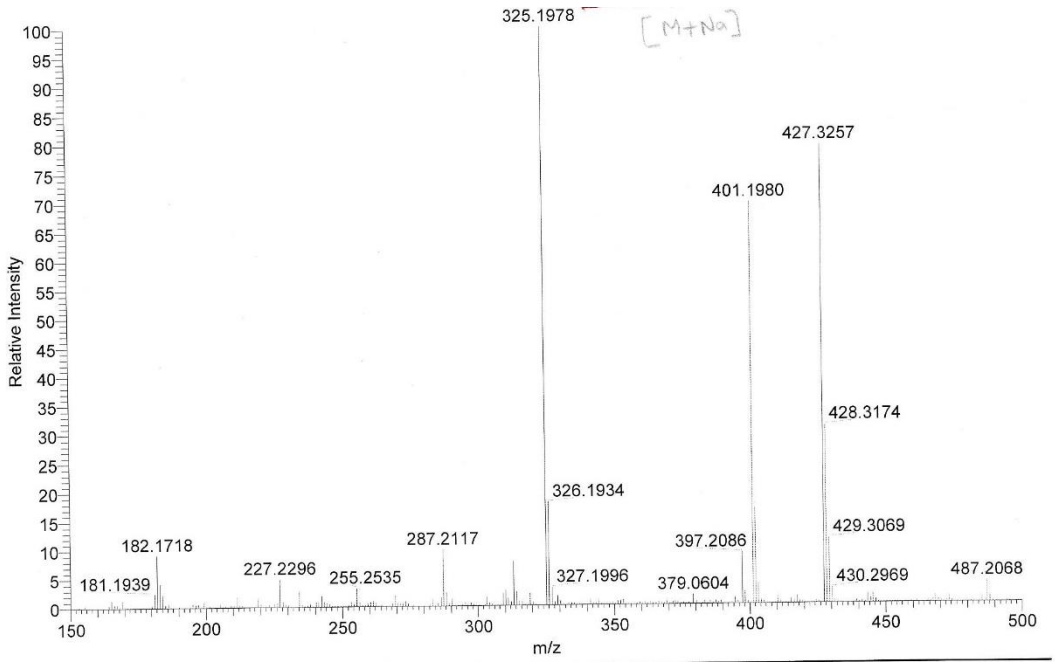
A. 112 IR spectrum of **(4.31)**



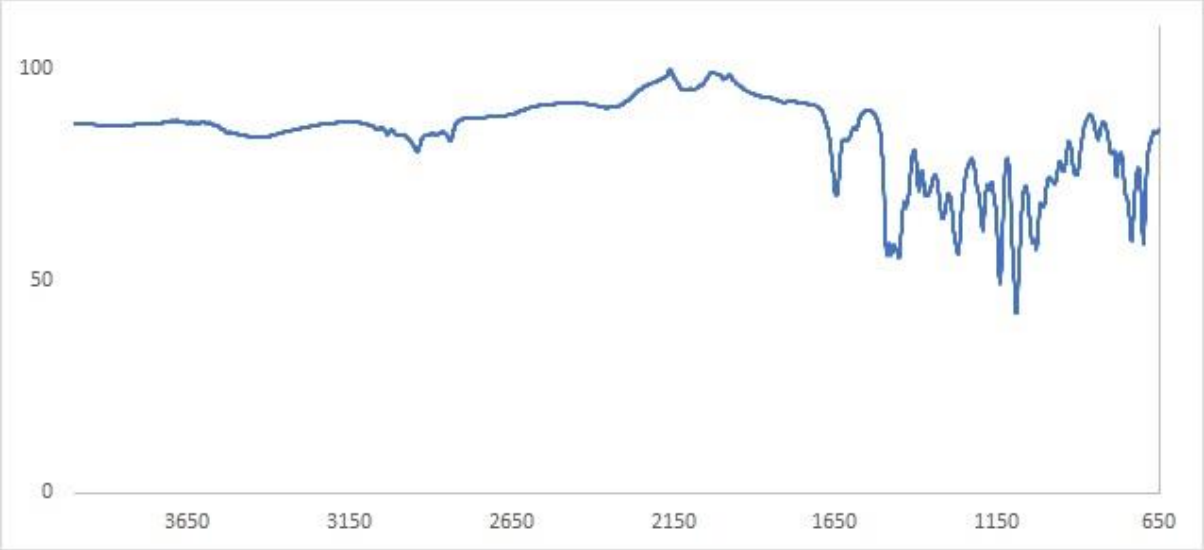
A. 113 ^{1}H NMR spectrum of **(4.12)**



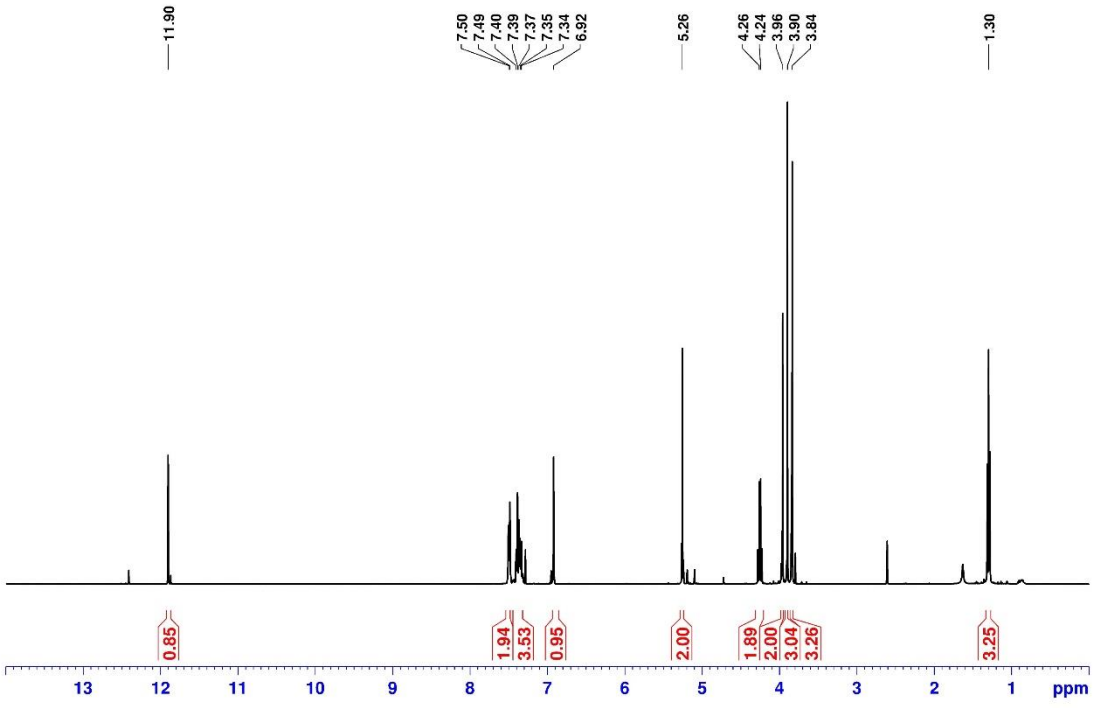
A. 114 ^{13}C NMR spectrum of **(4.12)**



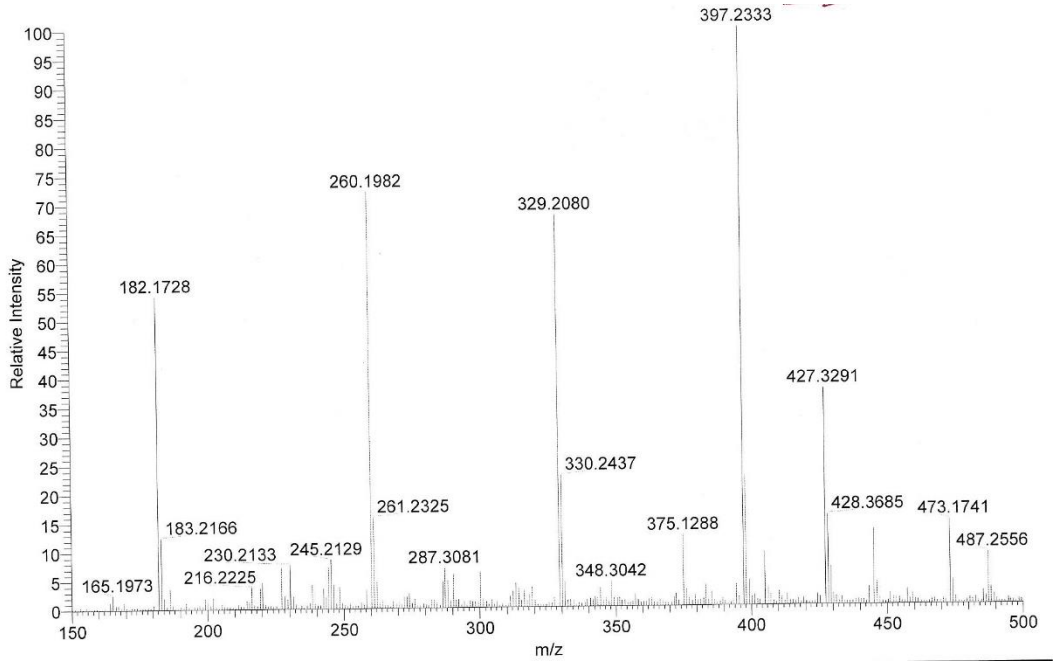
A. 115 ESI-MS of **(4.12)**, positive mode m/z 325 $[M+Na]^+$



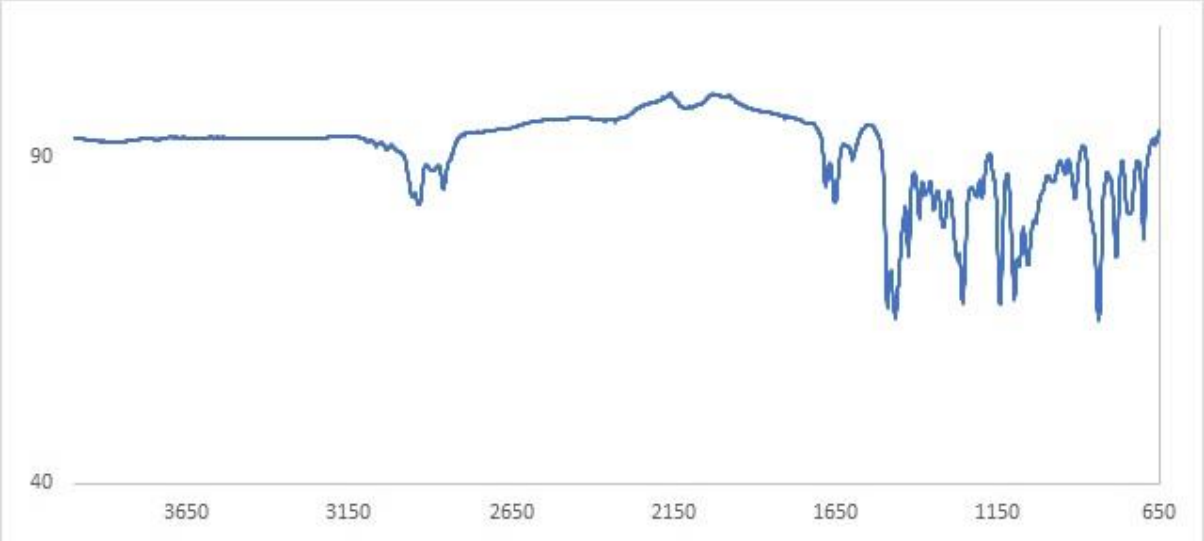
A. 116 IR spectrum of **(4.12)**



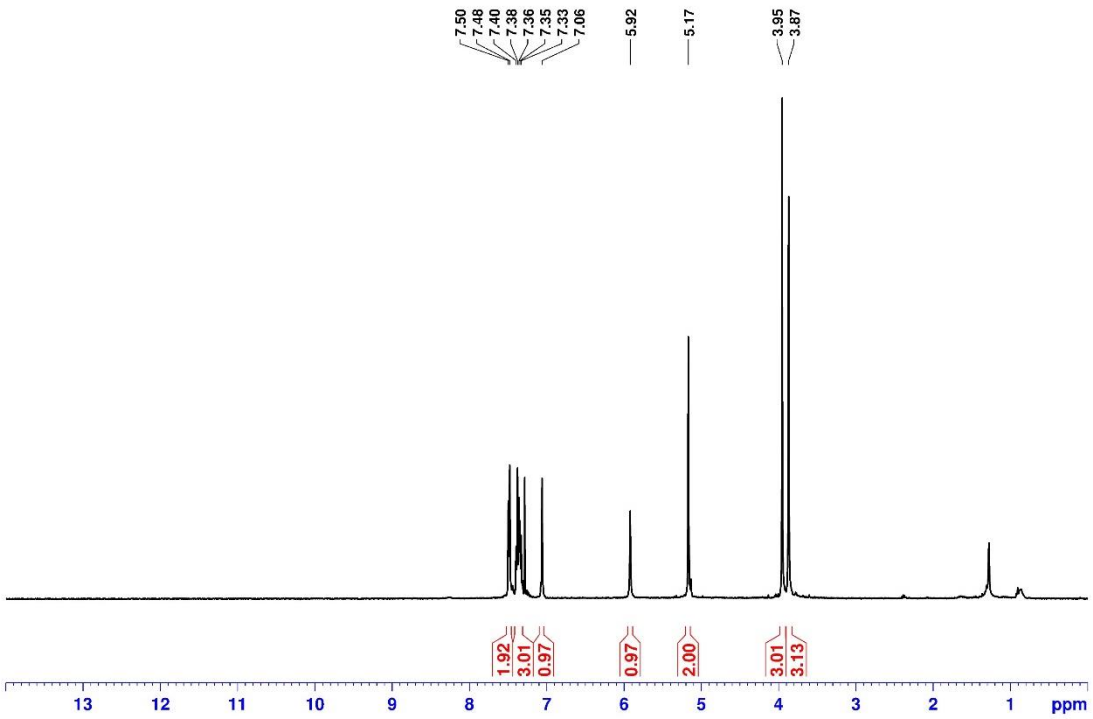
A. 117 ^{1}H NMR spectrum of **(4.32)**



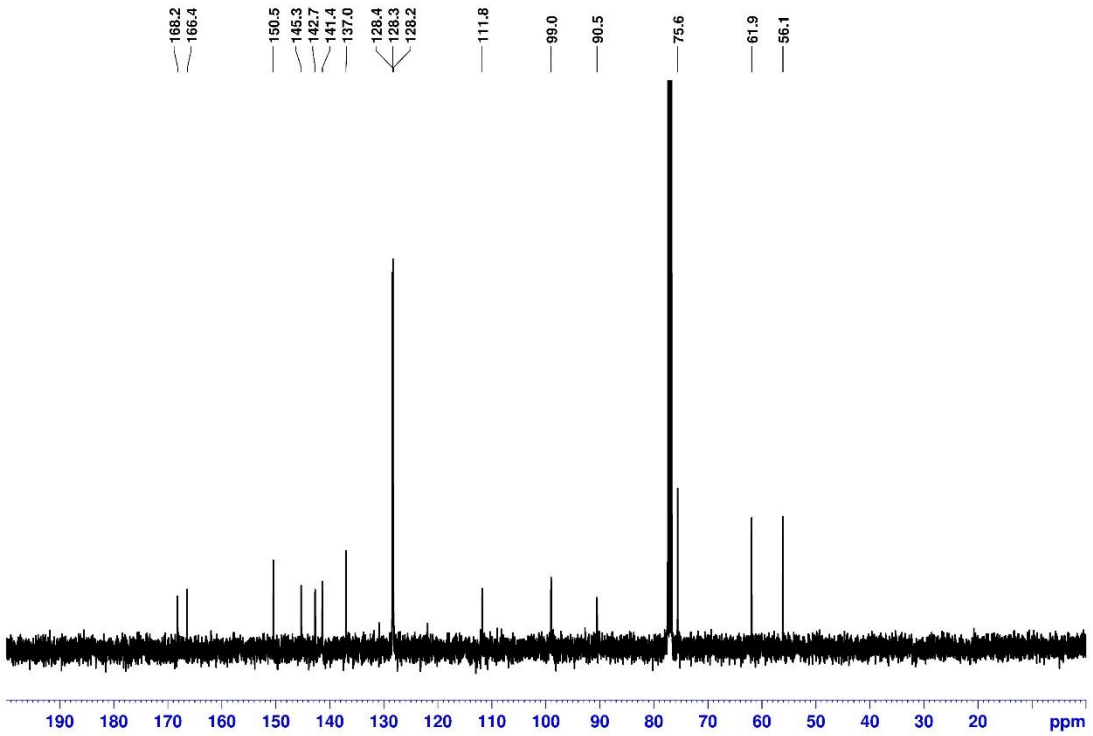
A. 118 ESI-MS of **(4.32)**, positive mode m/z 397 $[M+Na]^+$



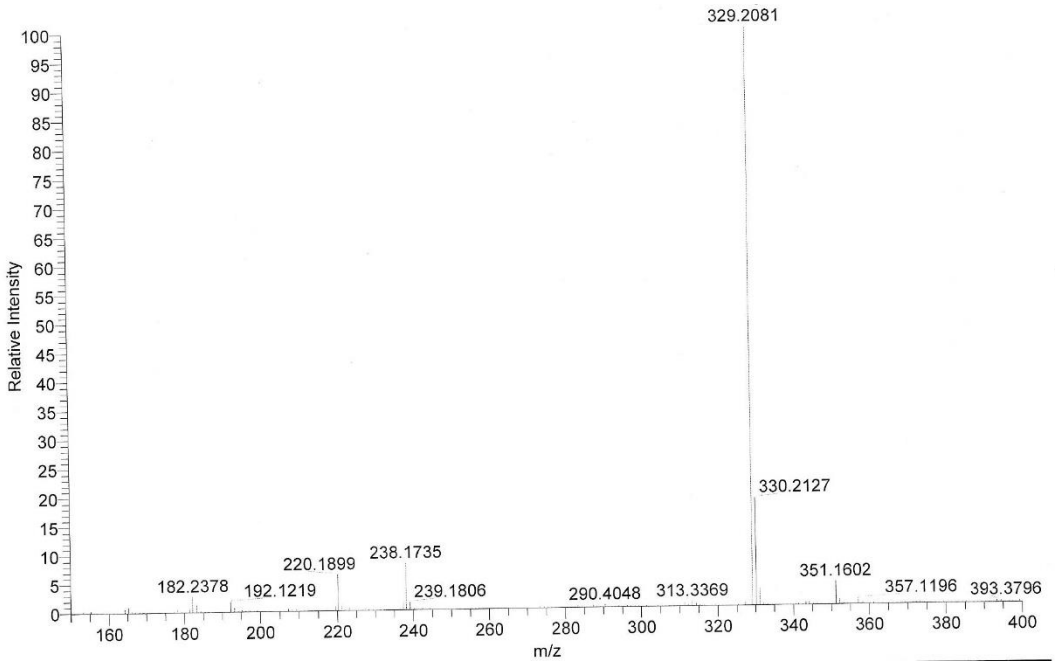
A. 119 IR spectrum of **(4.32)**



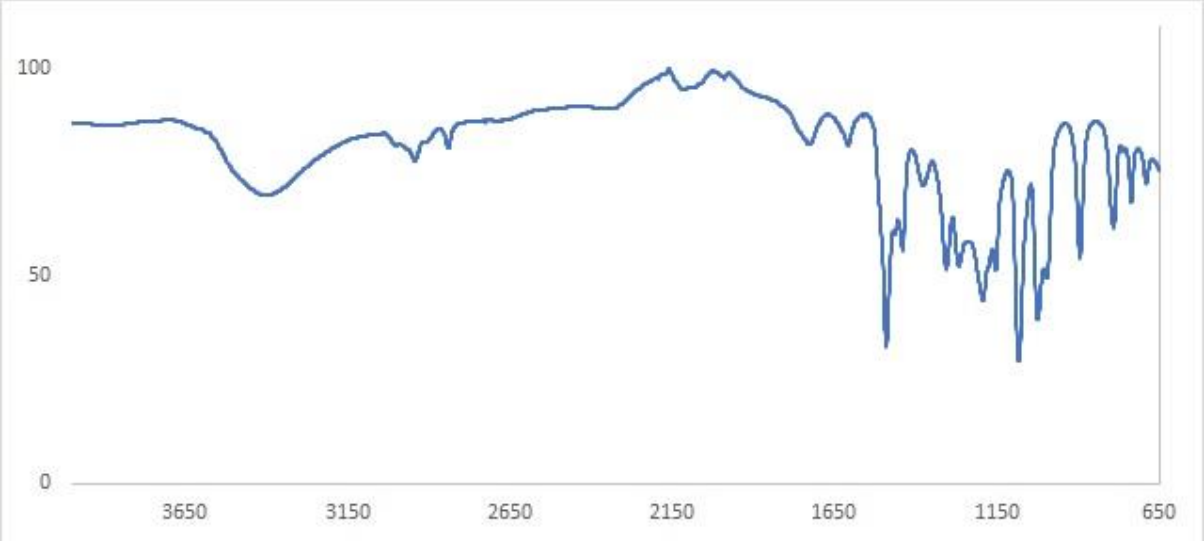
A. 120 ^{1}H NMR spectrum of **(4.19)**



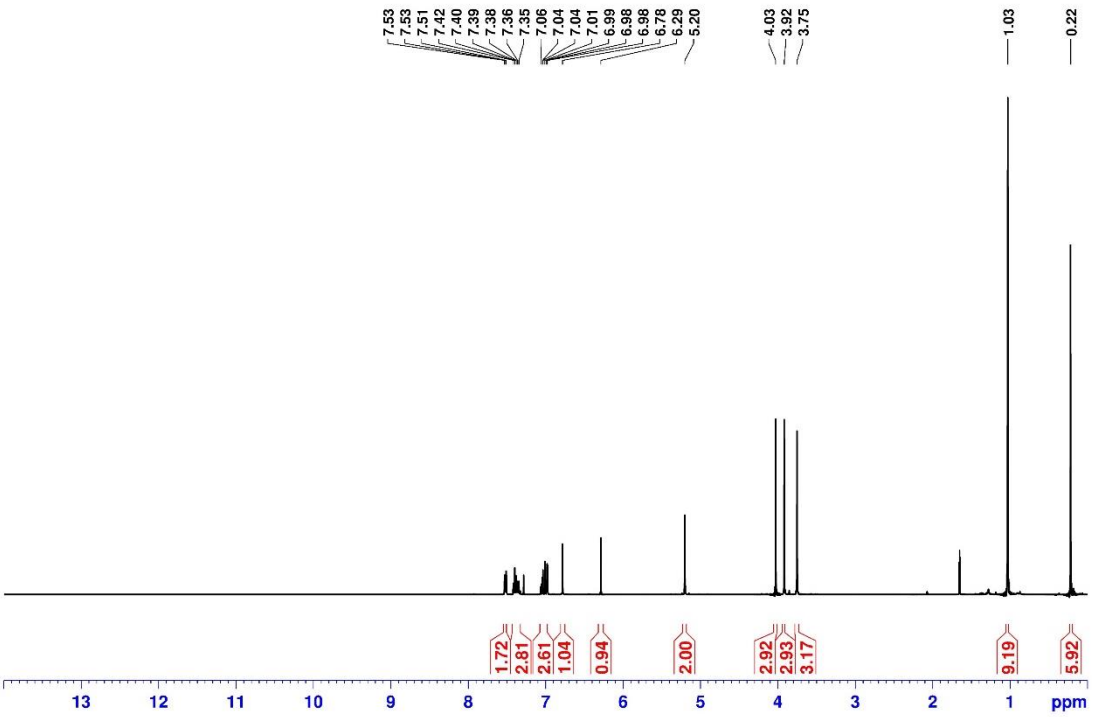
A. 121 ^{13}C NMR spectrum of **(4.19)**



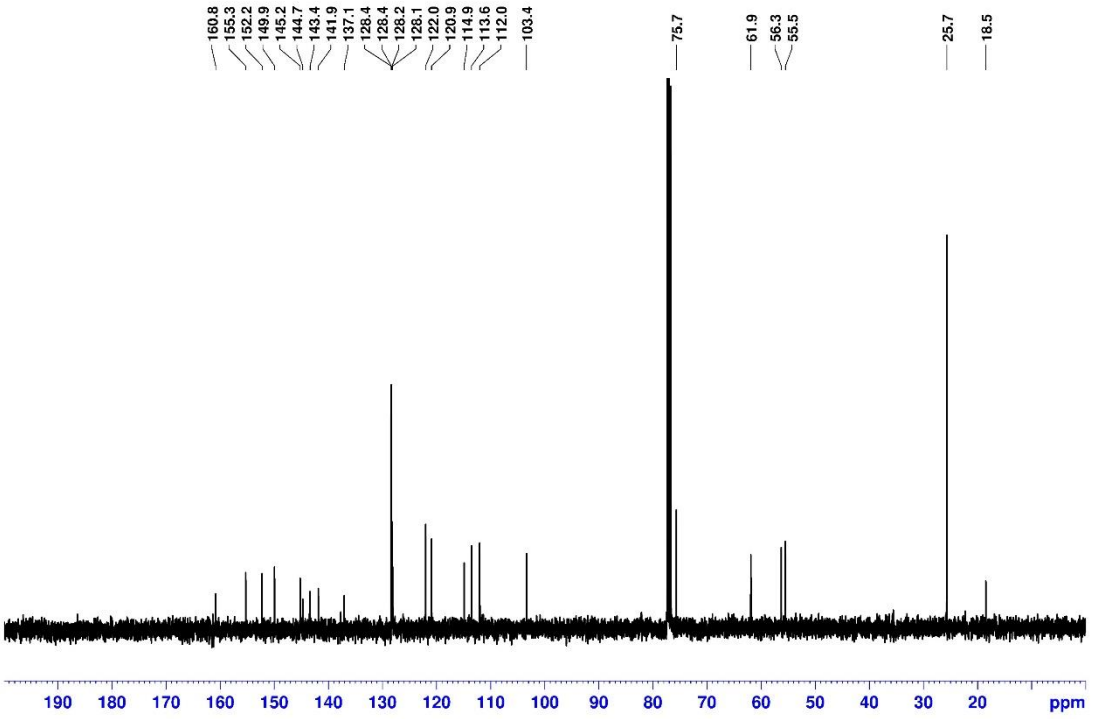
A. 122 ESI-MS of **(4.19)**, positive mode m/z 329 $[M+H]^+$



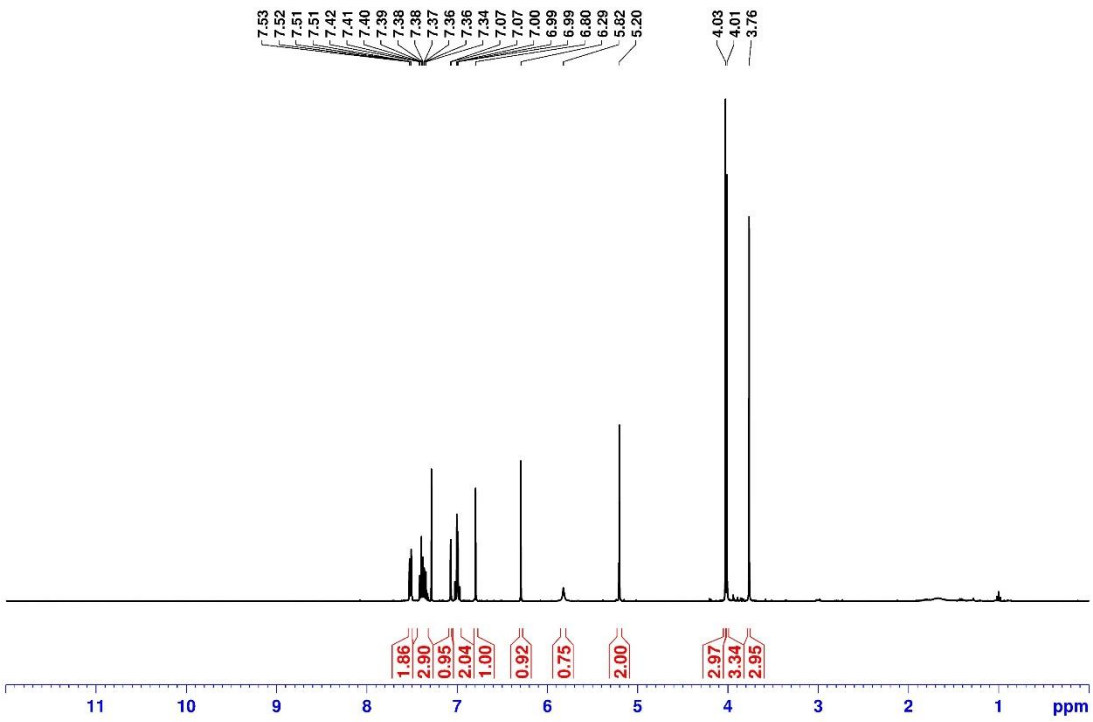
A. 123 IR spectrum of **(4.19)**



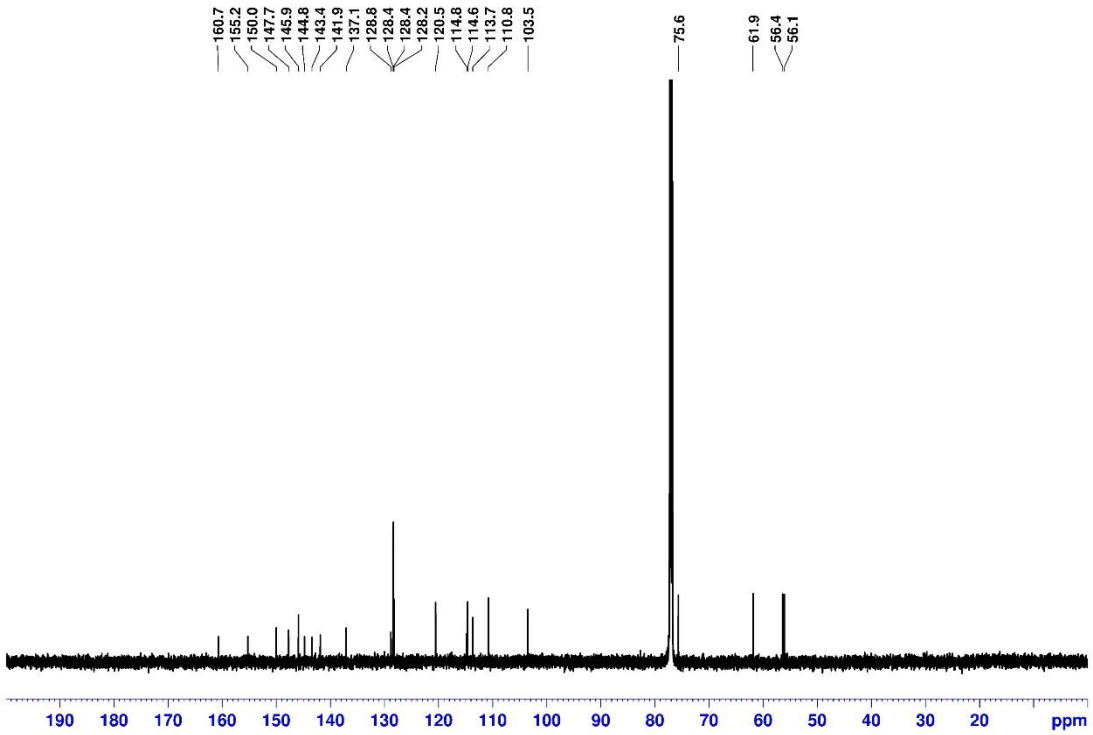
A. 124 ^{1}H NMR spectrum of **(4.35)**



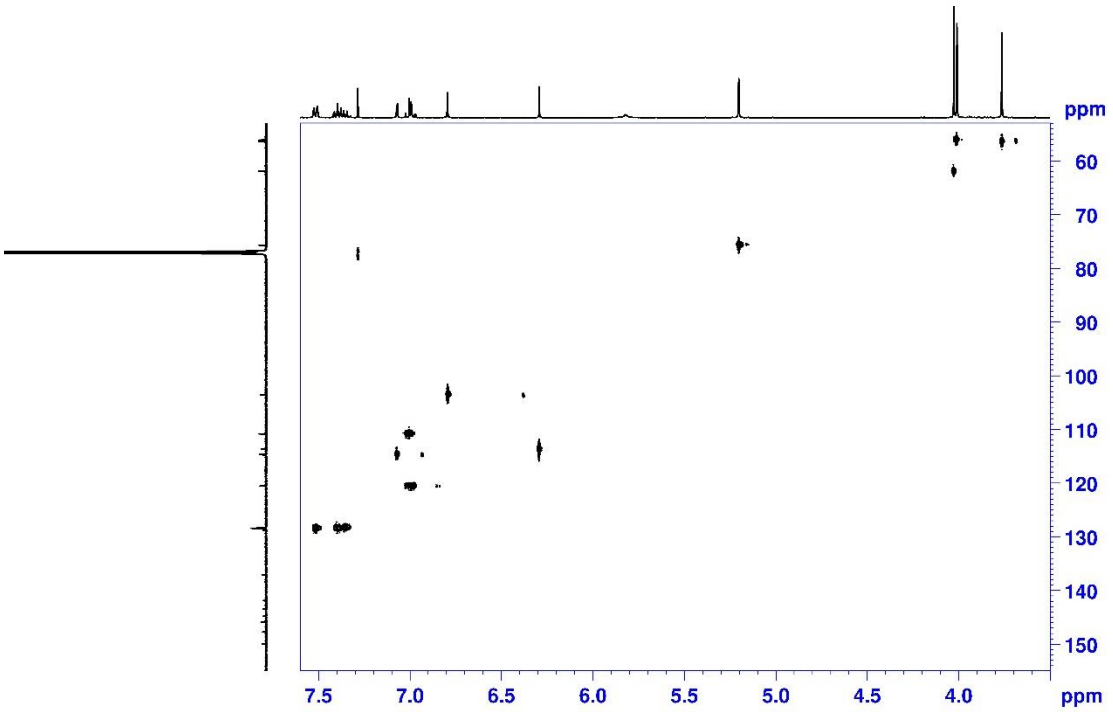
A. 125 ^{13}C NMR spectrum of **(4.35)**



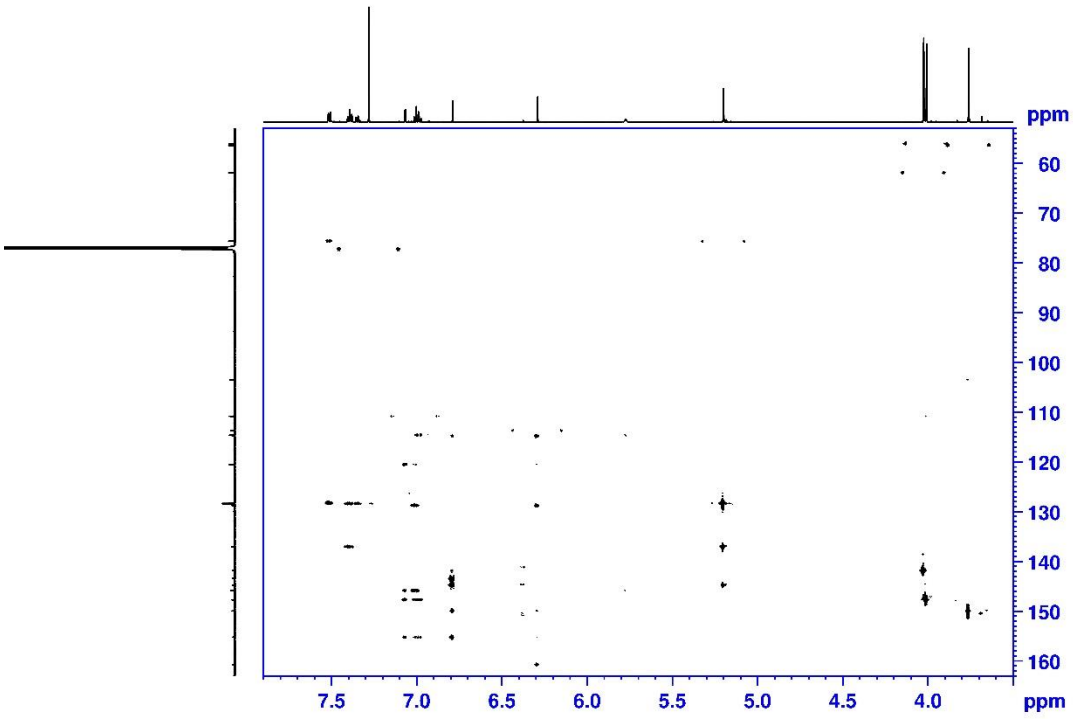
A. 126 ^{1}H NMR spectrum of **(4.36)**



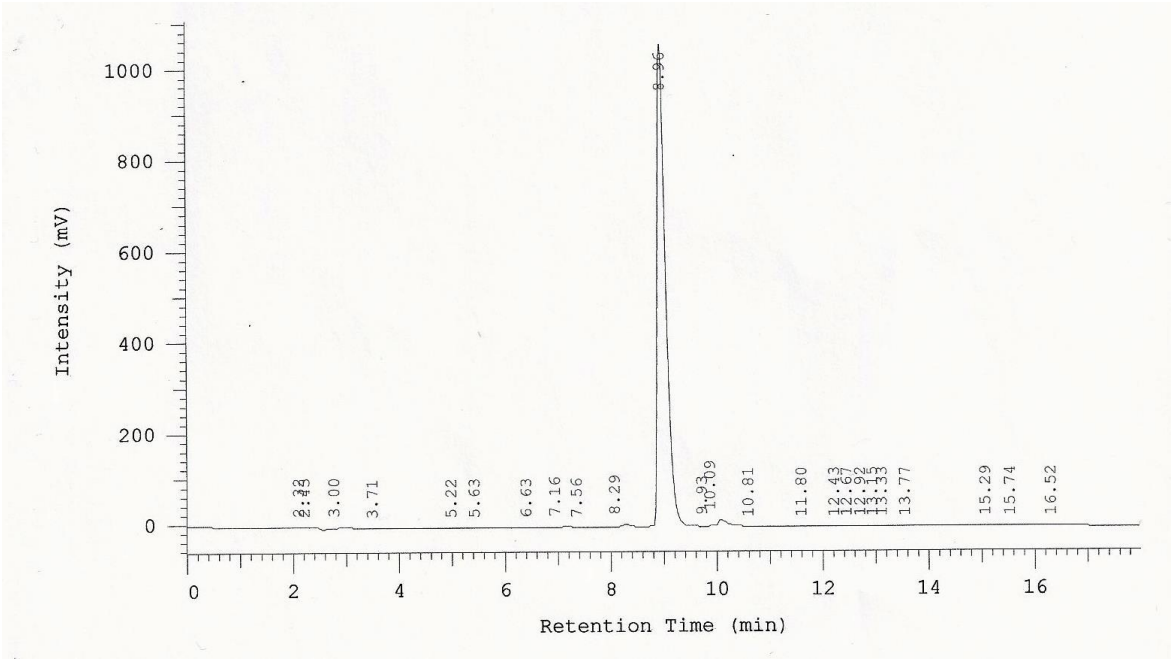
A. 127 ^{13}C NMR spectrum of **(4.36)**



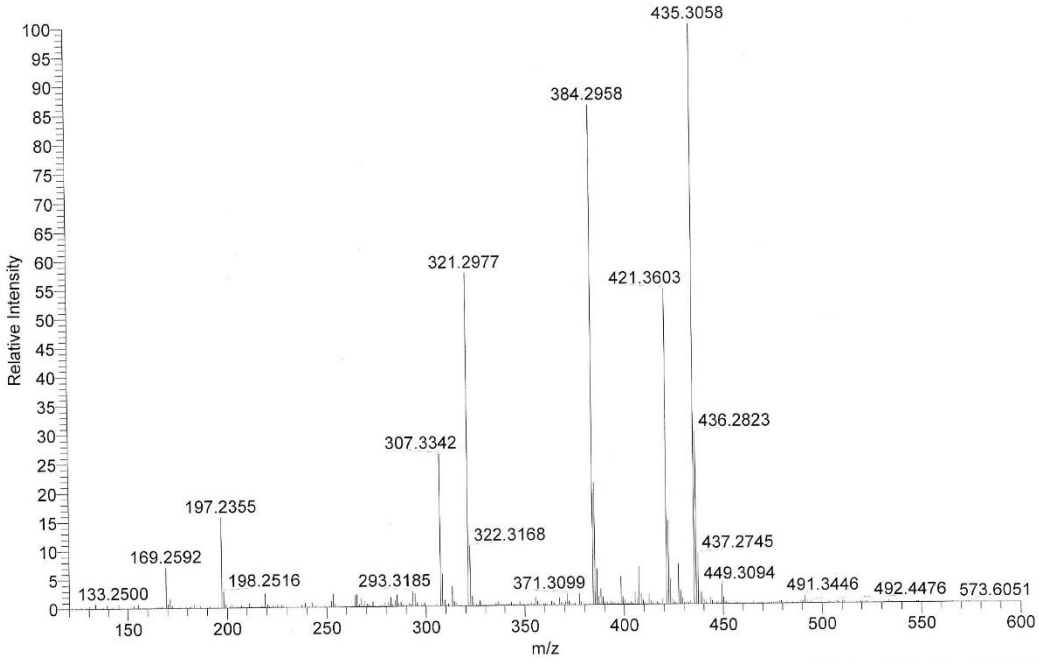
A. 128 HSQC spectrum of **(4.36)**



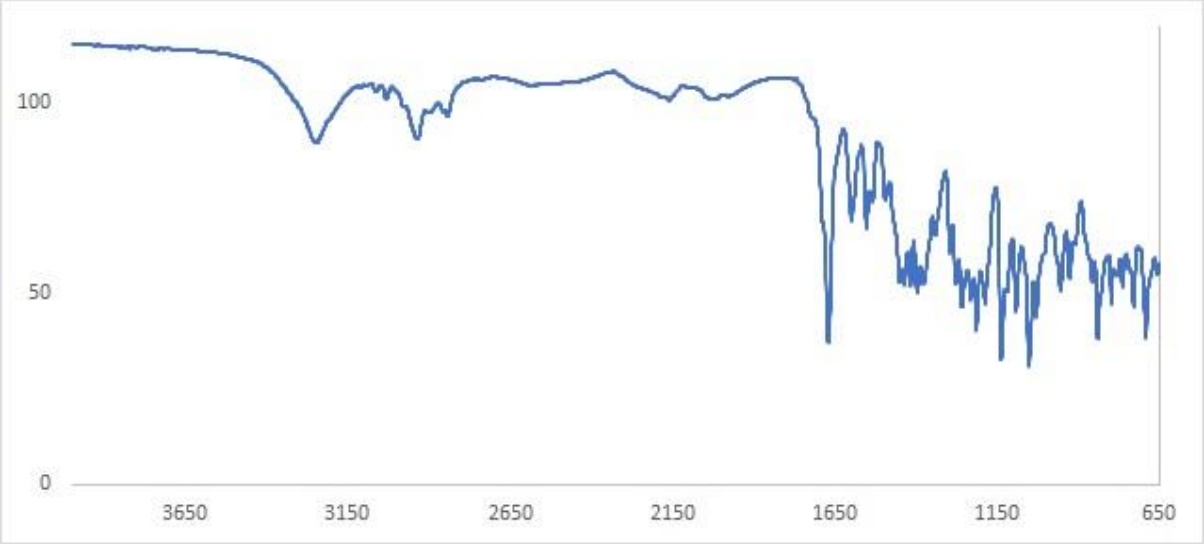
A. 129 HMBC spectrum of **(4.36)**



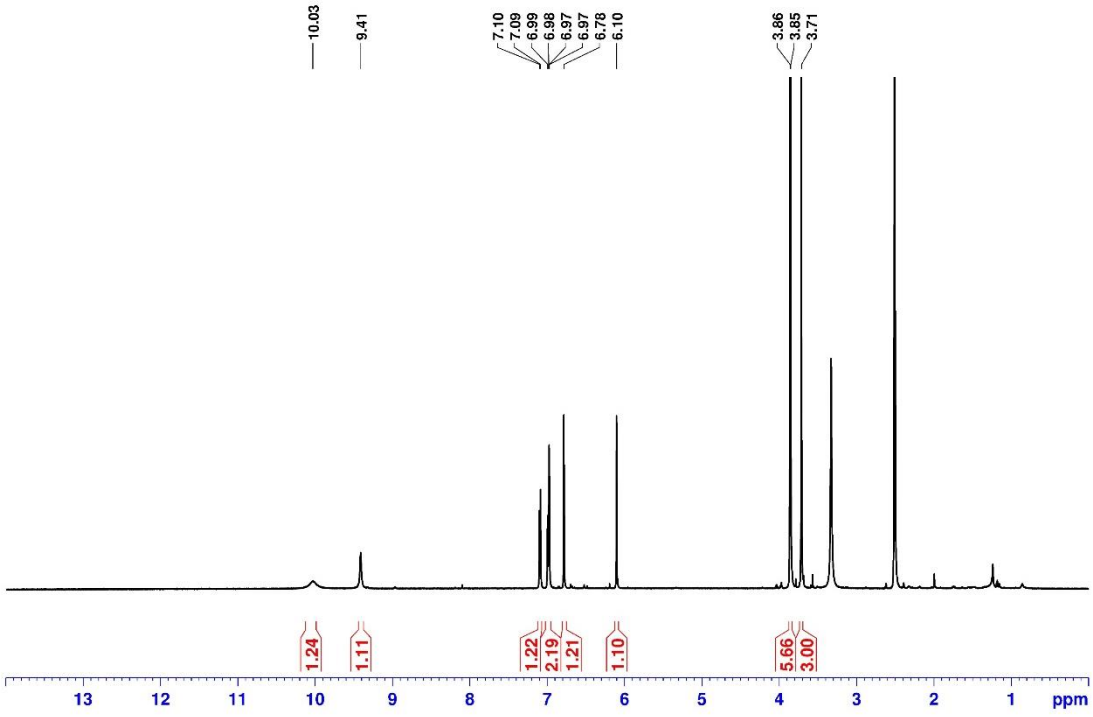
A. 130 HPLC chromatogram of **(4.36)**



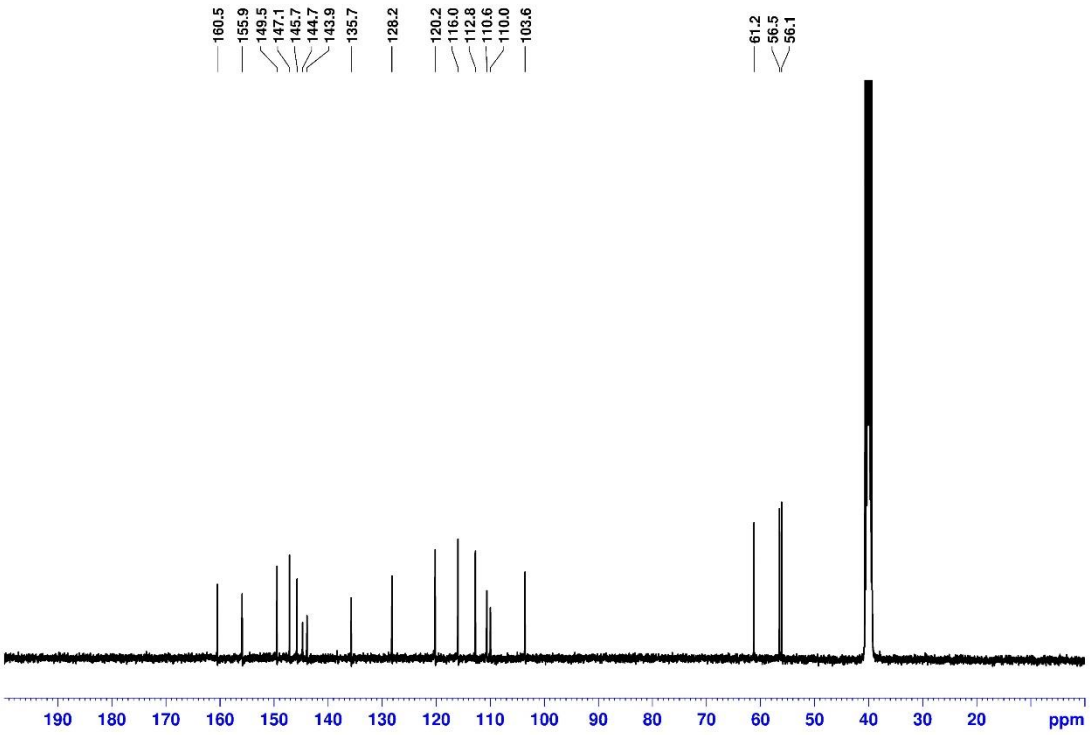
A. 131 ESI-MS of **(4.36)**, positive mode m/z 435 $[M+H]^+$



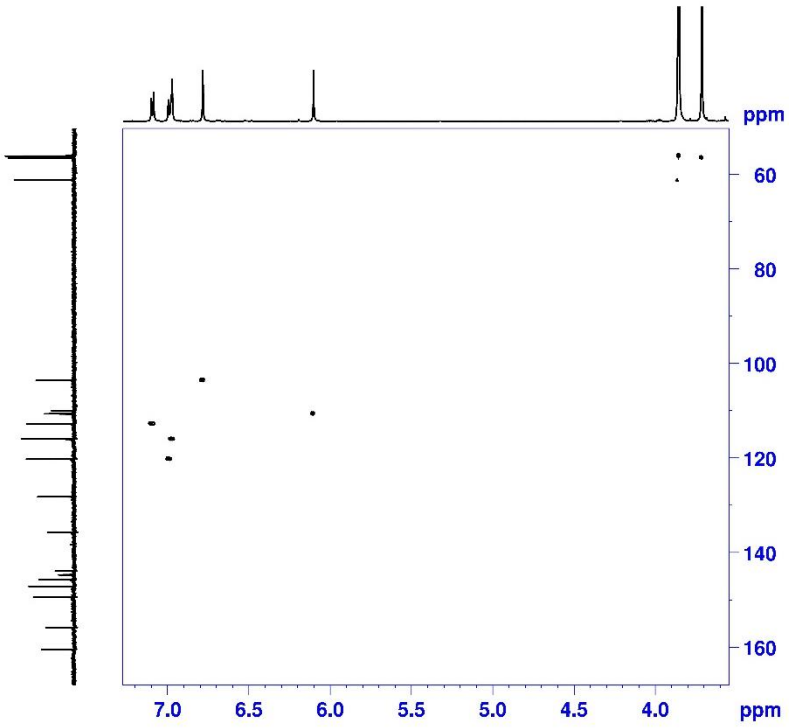
A. 132 IR spectrum of **(4.36)**



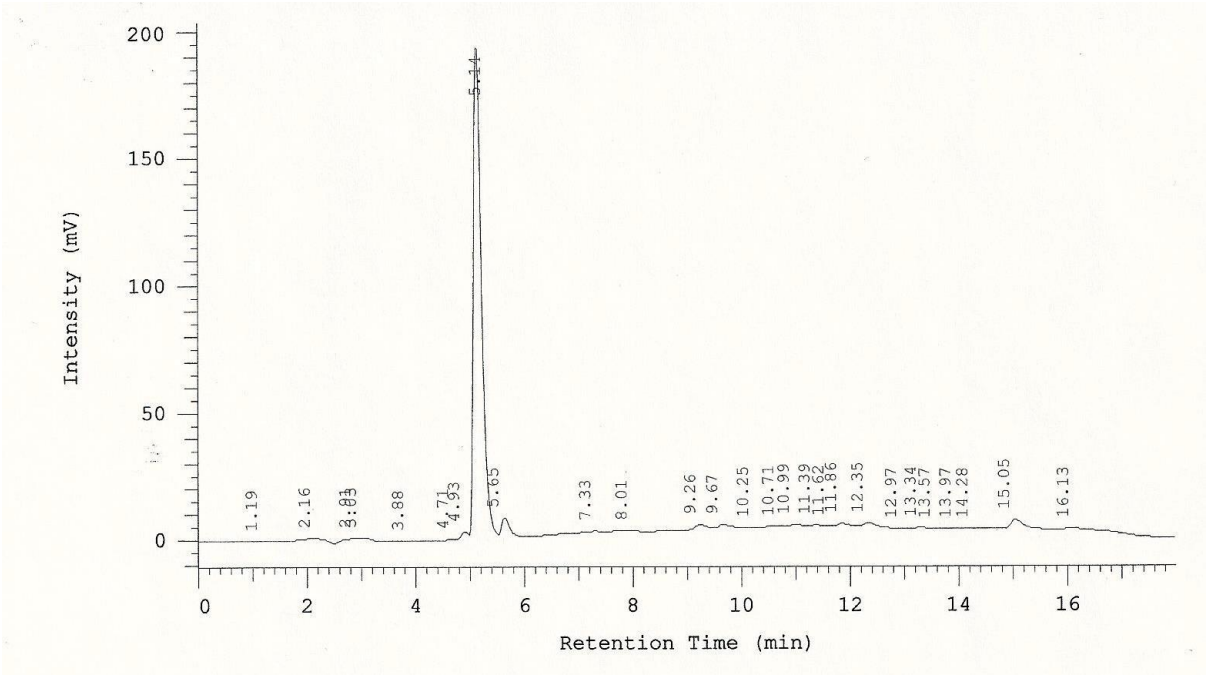
A. 133 ^{1}H NMR spectrum of **(4.37)**



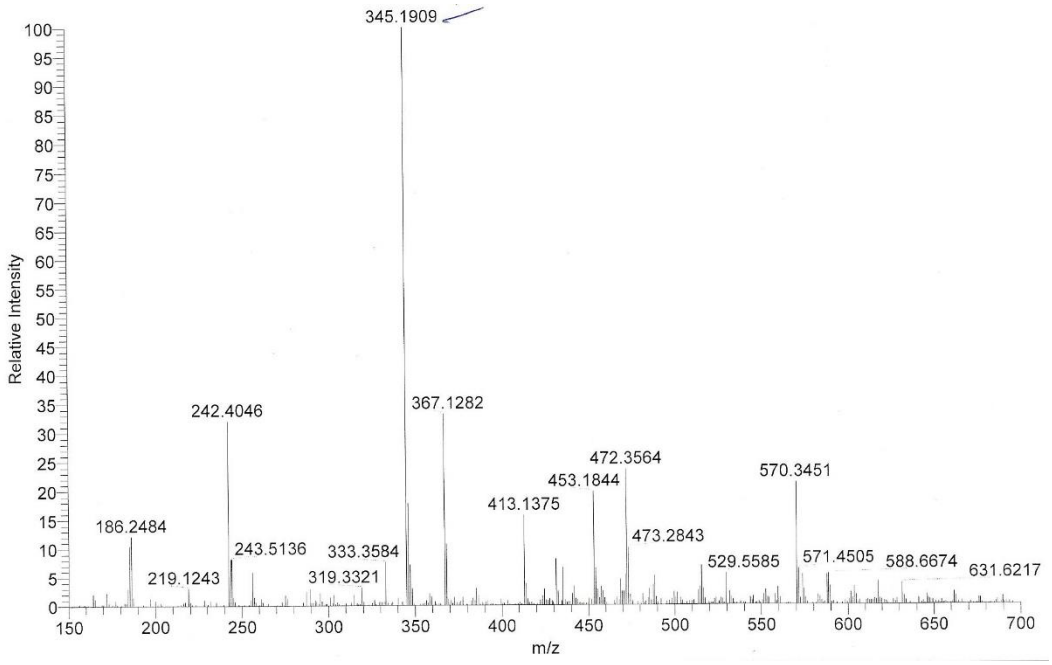
A. 134 ^{13}C NMR spectrum of **(4.37)**



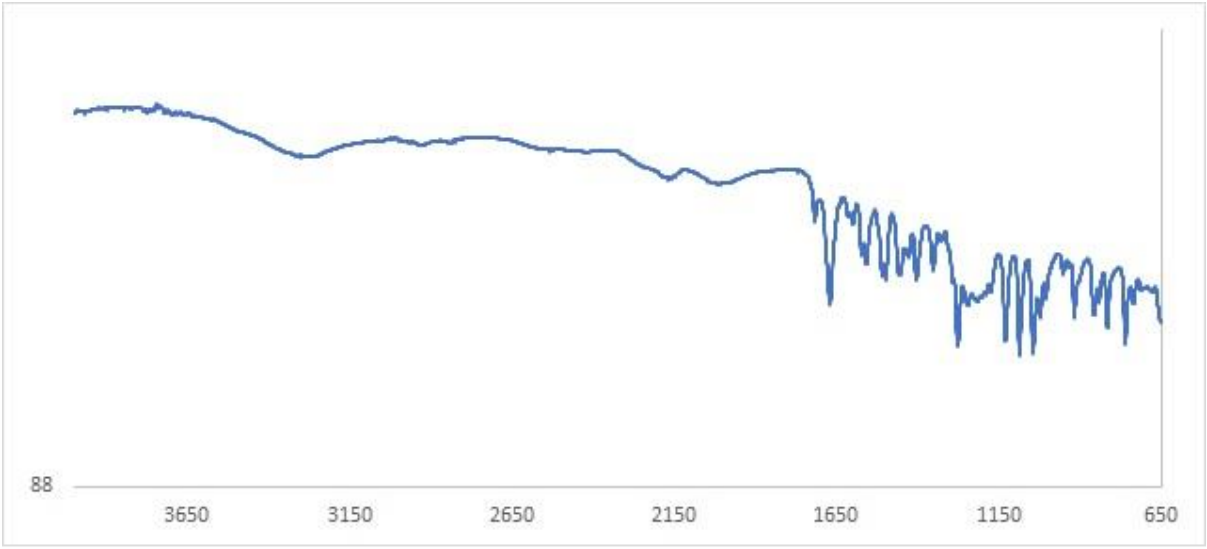
A. 135 HSQC spectrum of **(4.37)**



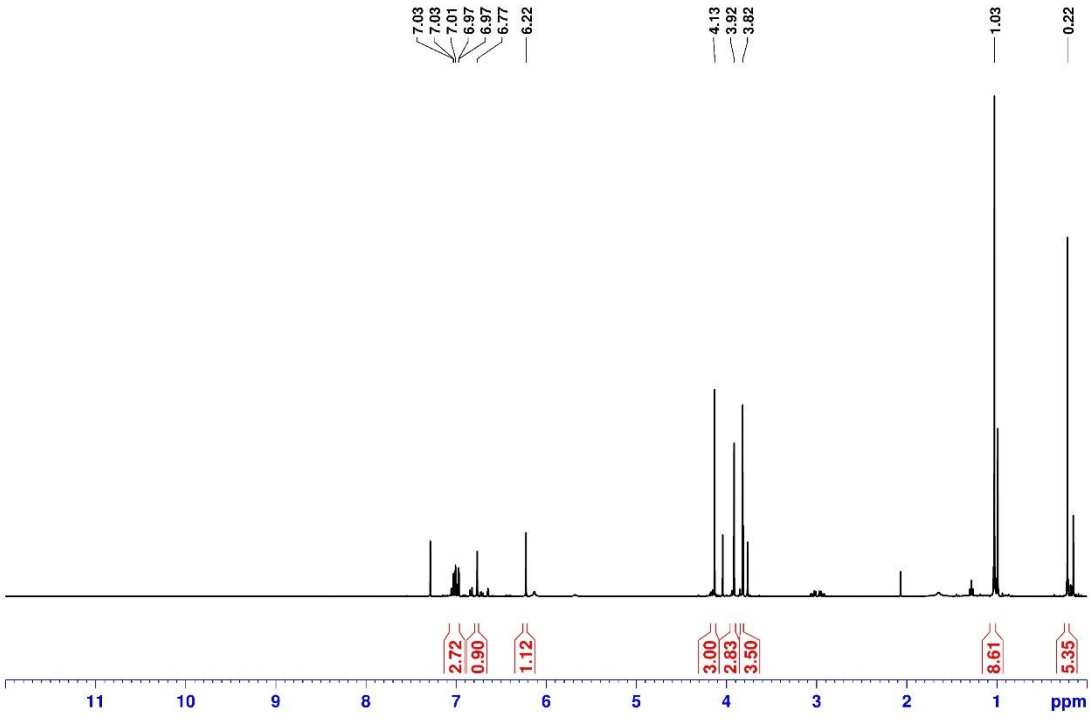
A. 136 HPLC chromatogram of **(4.37)**



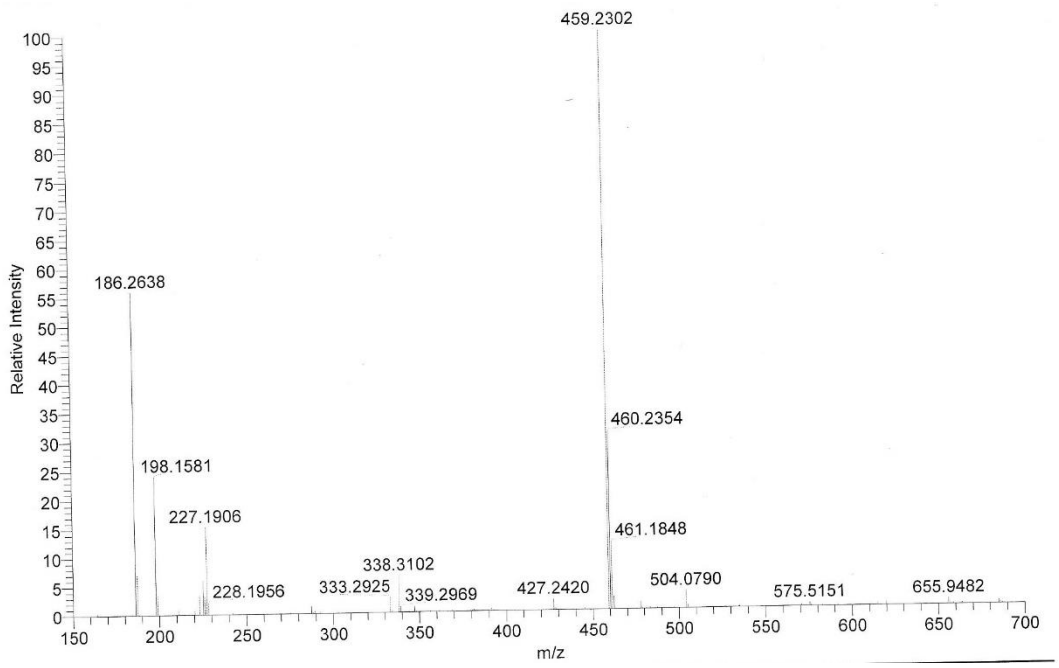
A. 137 ESI-MS of **(4.37)**, positive mode m/z 345 $[M+H]^+$



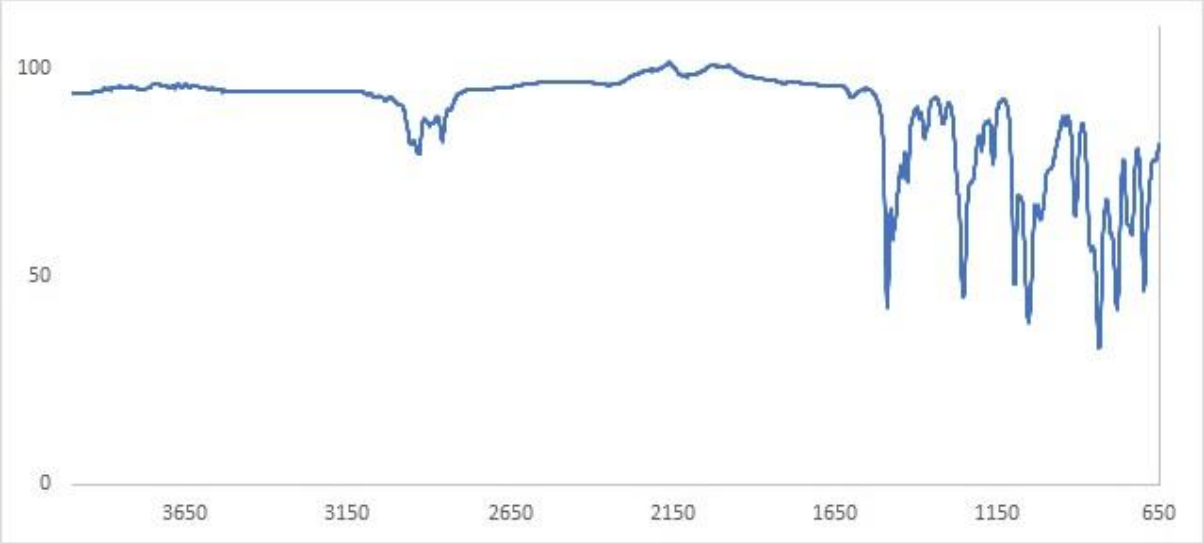
A. 138 IR spectrum of **(4.37)**



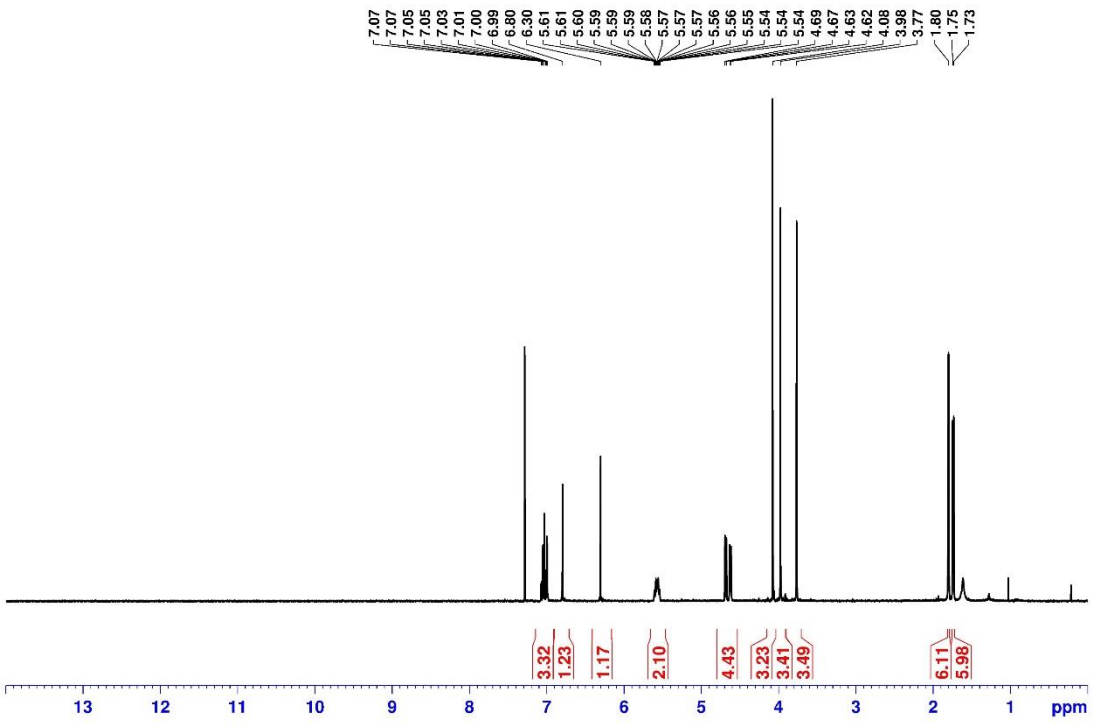
A. 139 ^{1}H NMR spectrum of **(4.38)**



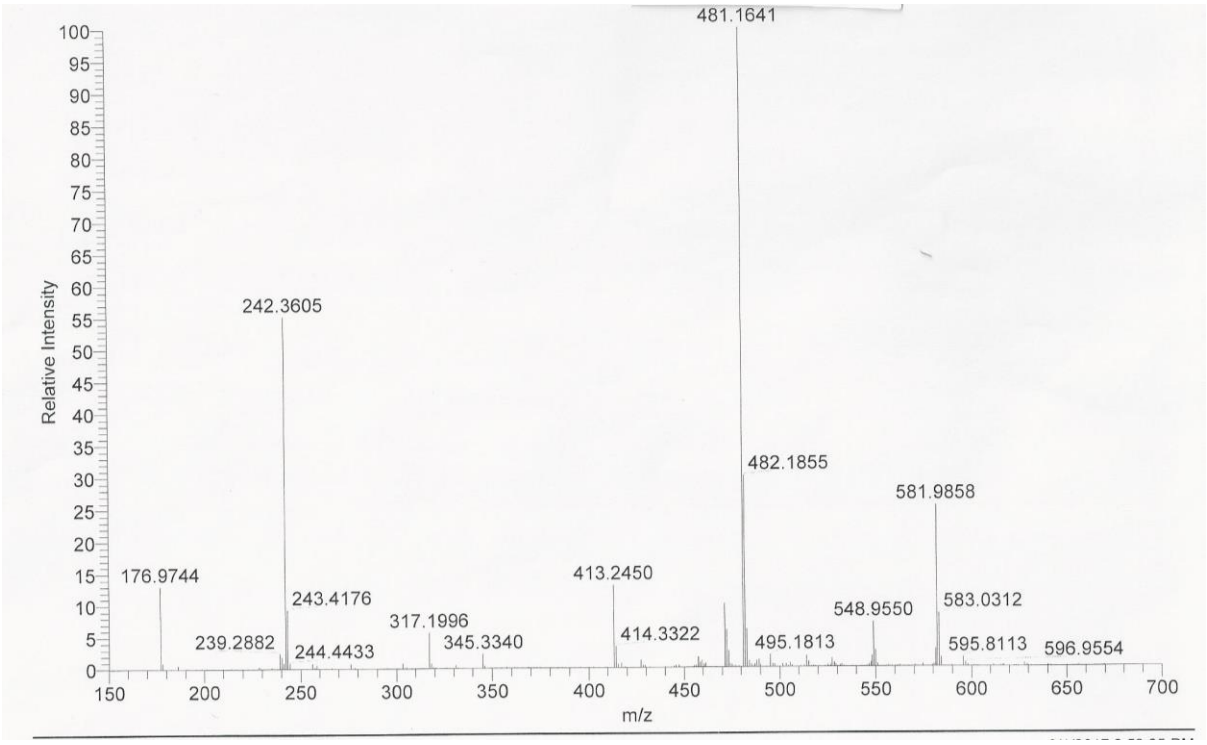
A. 140 ESI-MS of **(4.38)**, positive mode m/z 459 $[M+H]^+$



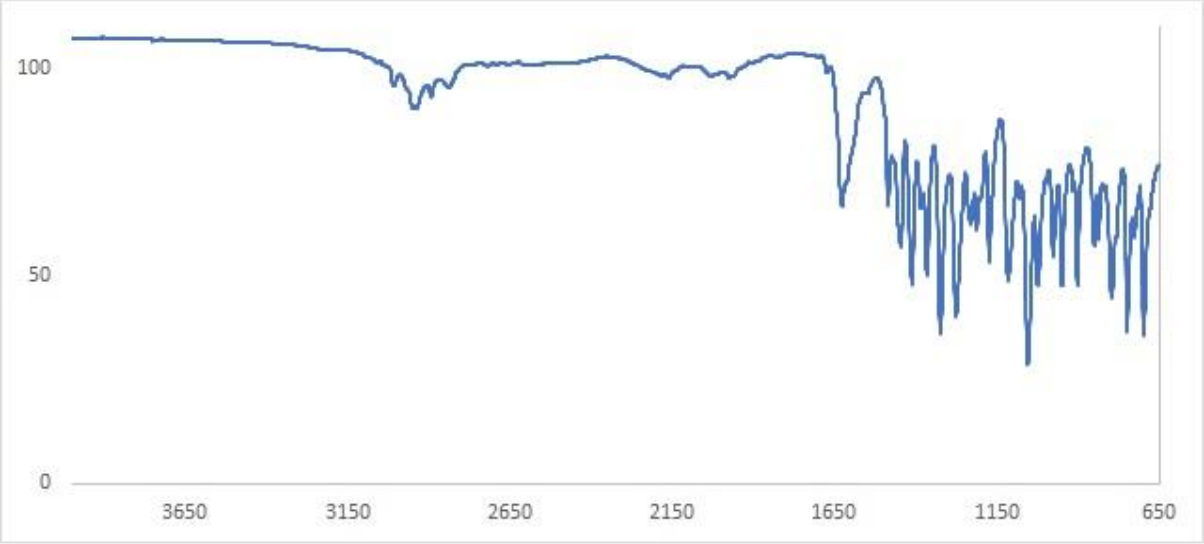
A. 141 IR spectrum of **(4.38)**



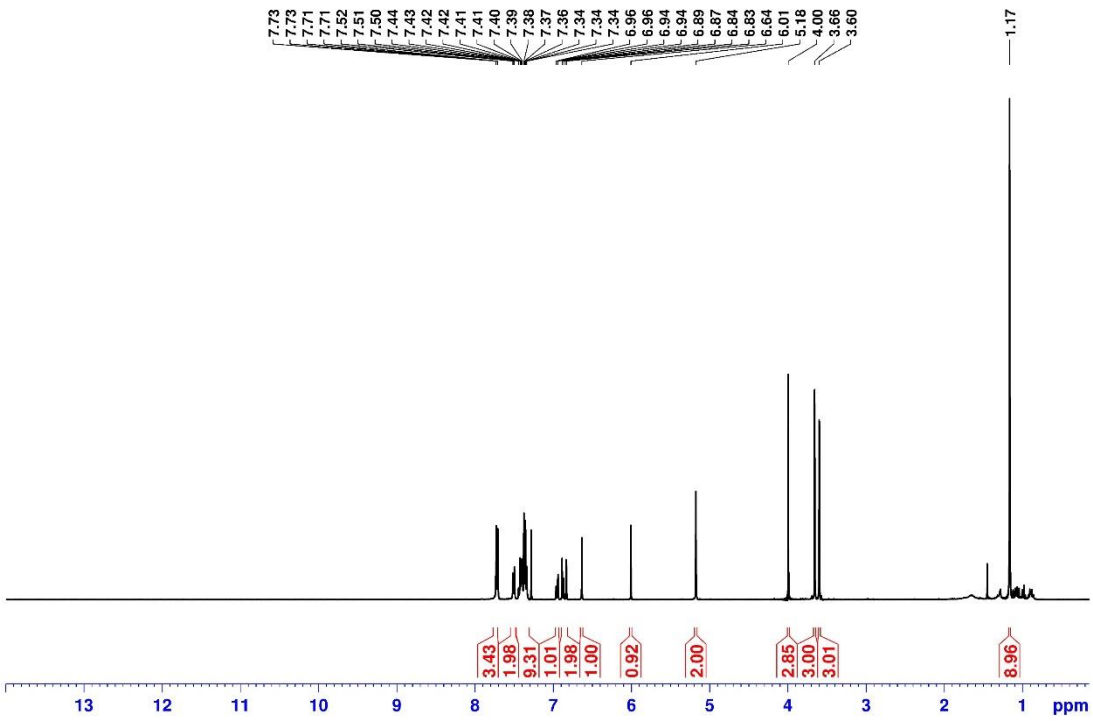
A. 142 ^{1}H NMR spectrum of **(4.40)**



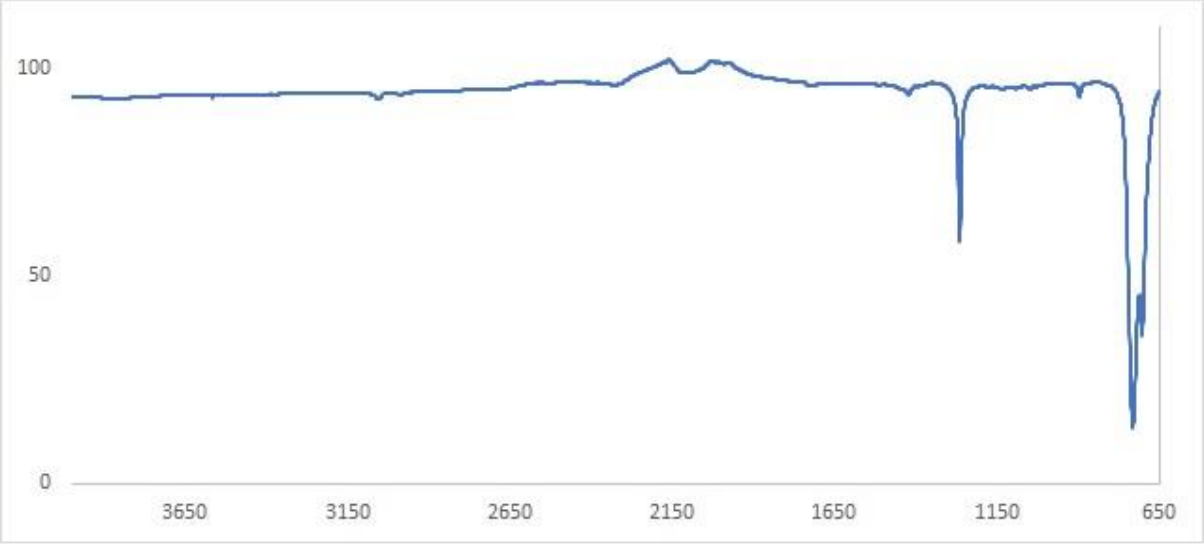
A. 143 ESI-MS of **(4.40)**, positive mode m/z 481 $[M+H]^{+}$



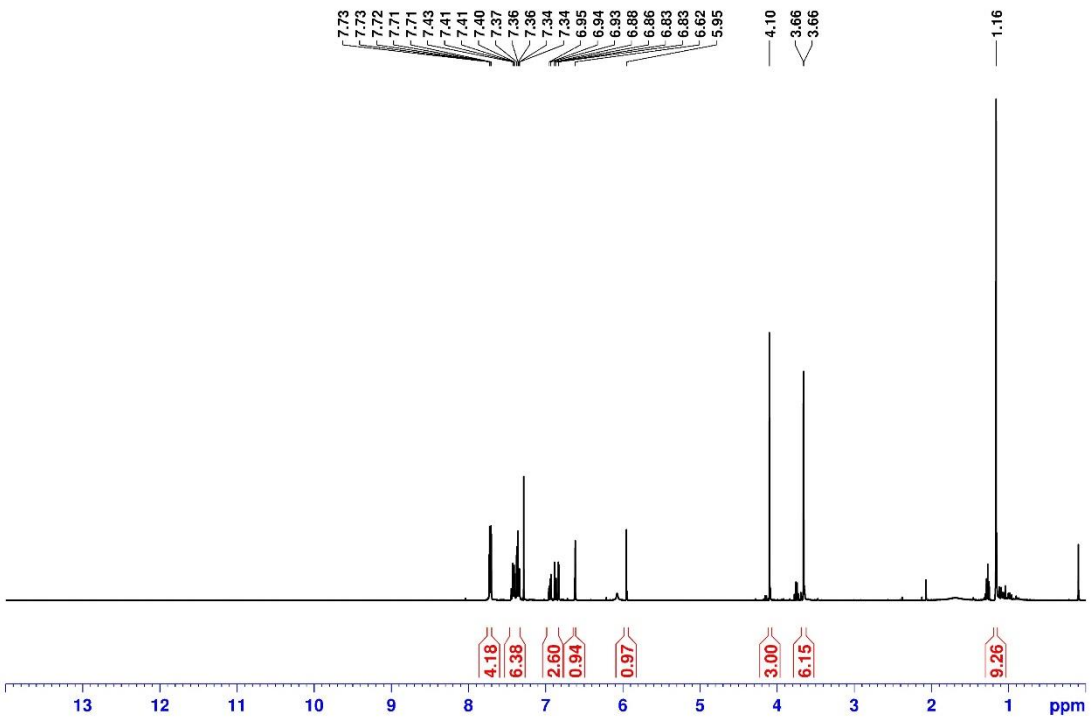
A. 144 IR spectrum of **(4.40)**



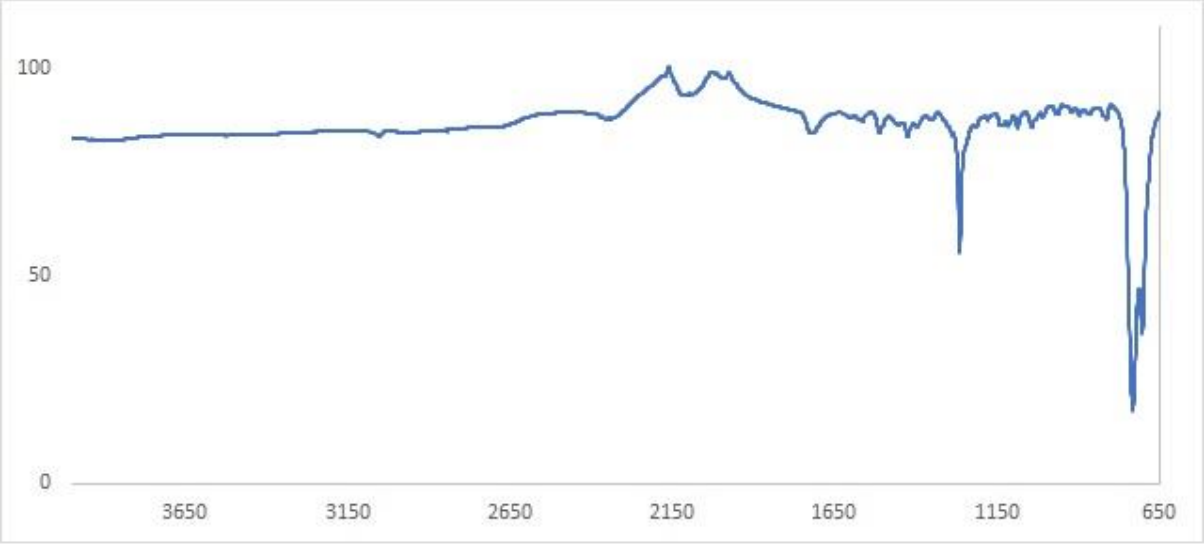
A. 145 ^{1}H NMR spectrum of **(4.41)**



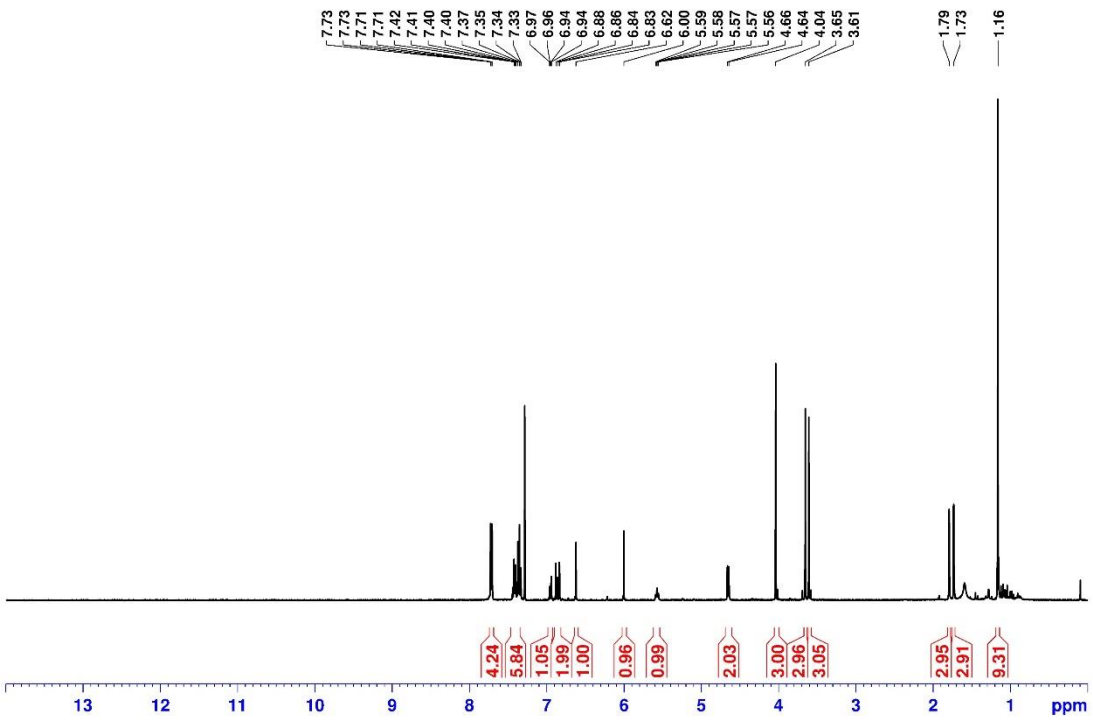
A. 146 IR spectrum of **(4.41)**



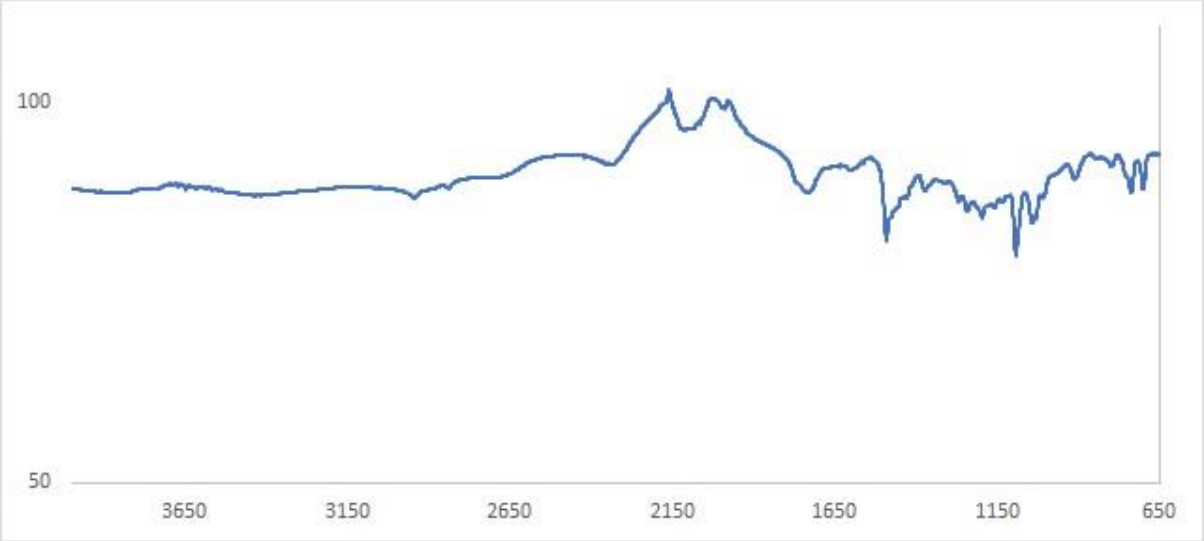
A. 147 ^{1}H NMR spectrum of **(4.42)**



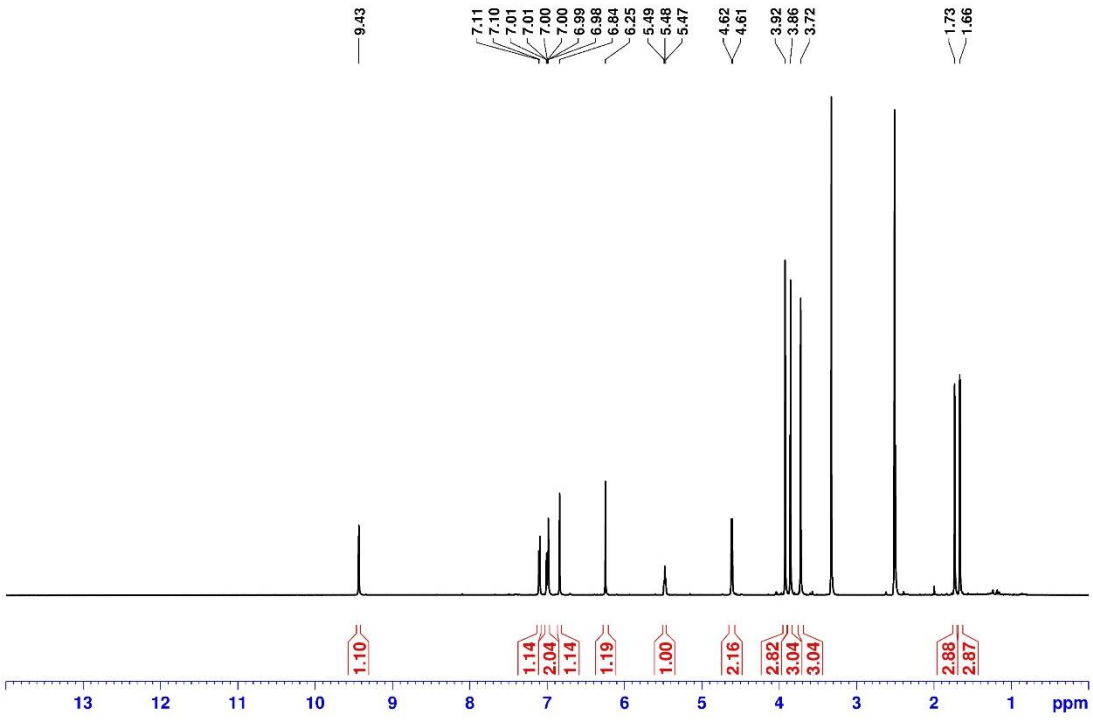
A. 148 IR spectrum of **(4.42)**



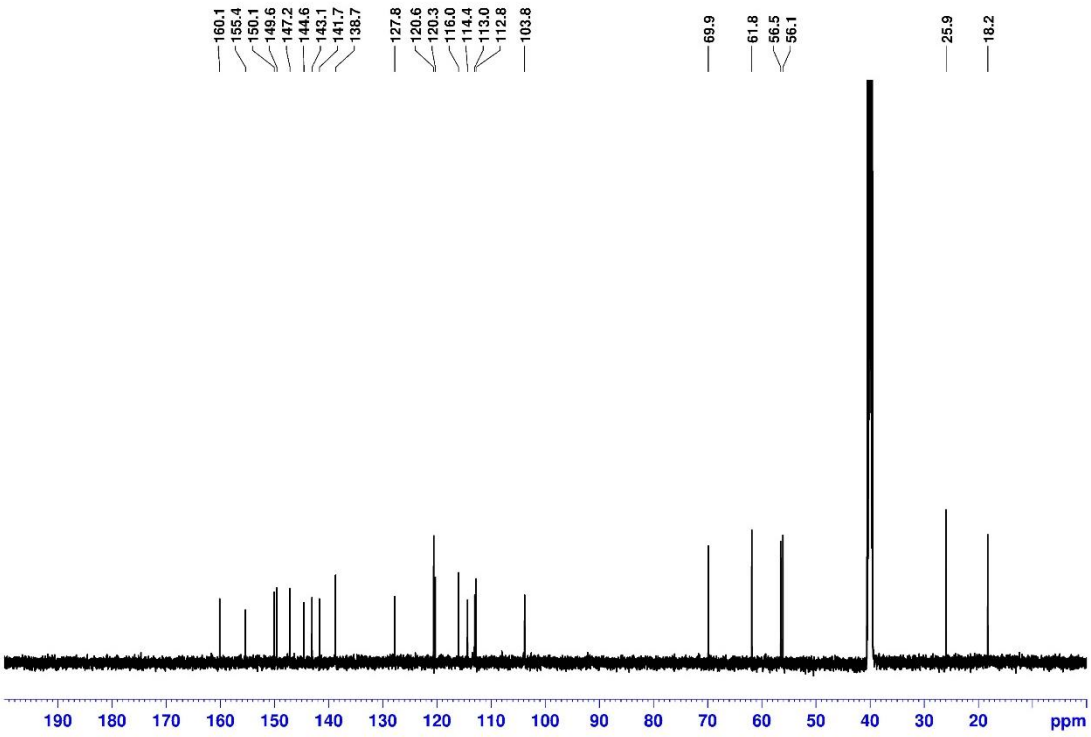
A. 149 ^{1}H NMR spectrum of **(4.43)**



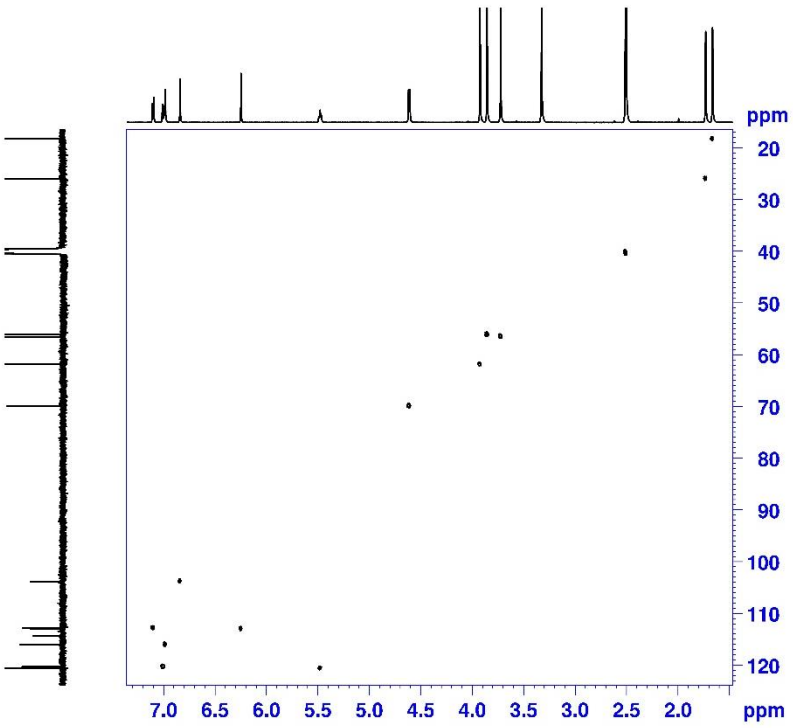
A. 150 IR spectrum of **(4.43)**



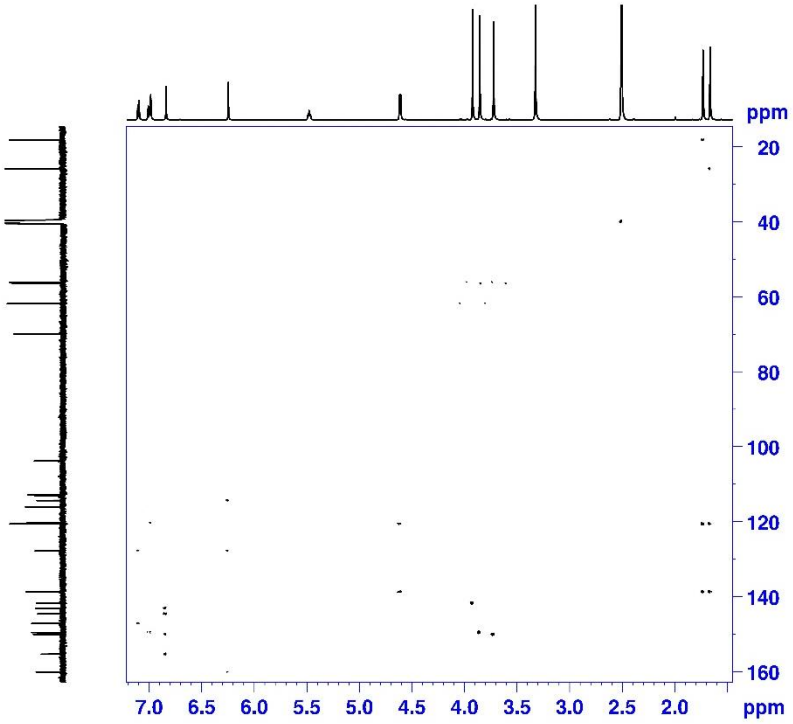
A. 151 ^{1}H NMR spectrum of **(4.44)**



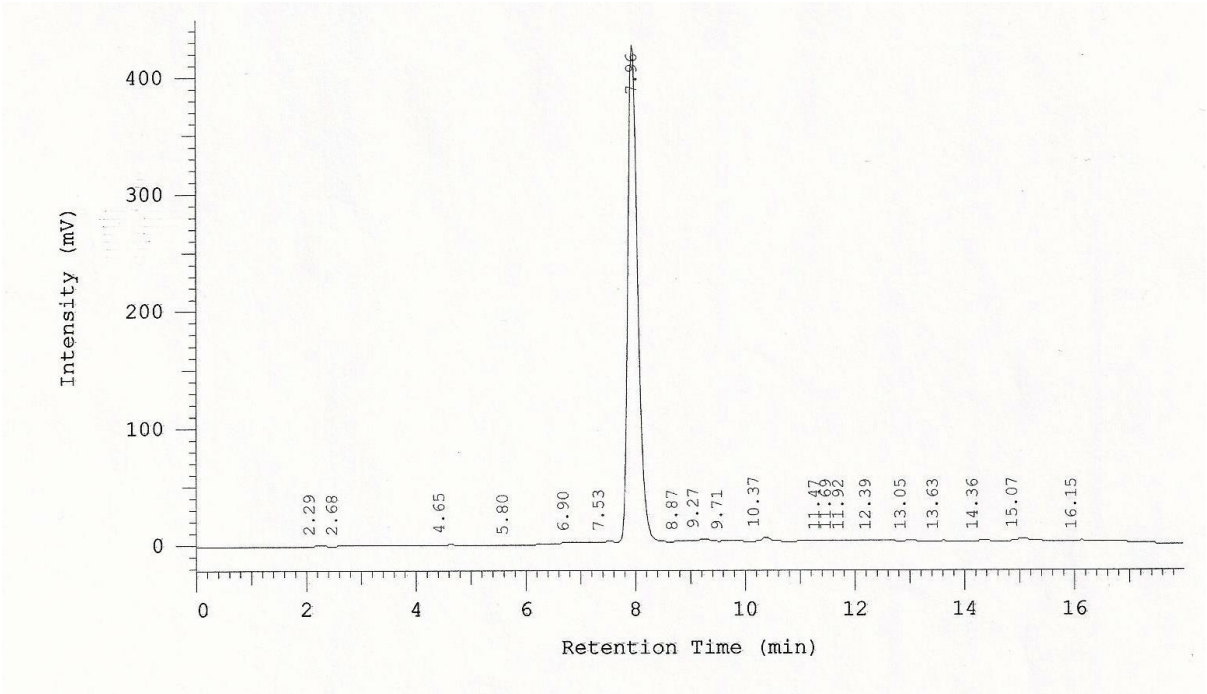
A. 152 ^{13}C NMR spectrum of **(4.44)**



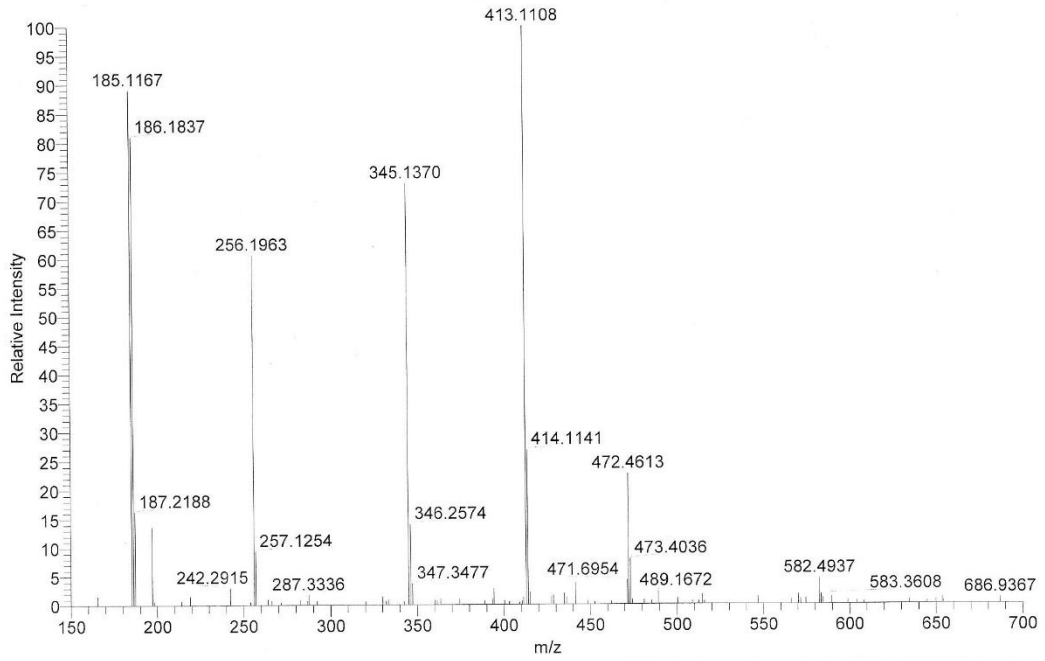
A. 153 HSQC spectrum of **(4.44)**



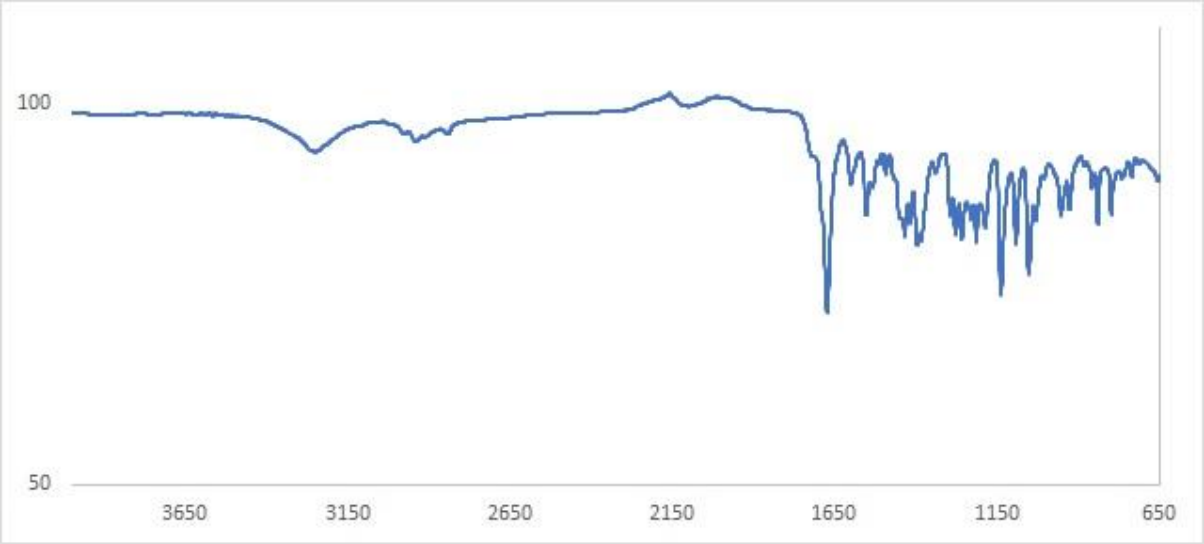
A. 154 HMBC spectrum of **(4.44)**



A. 155 HPLC chromatogram of **(4.44)**



A. 156 ESI-MS of **(4.44)**, positive mode m/z 413 $[M+H]^+$



A. 157 IR spectrum of **(4.44)**