SUPPLEMENTARY MATERIALS

Mn(II) and Zn(II) Complexes of a Coumarin Derivative: Synthesis, Characterization and Biological Potential

Zulfiqar Ali Shahid, Rukhsana Tabassum*

Institute of Chemistry, Islamia University of Bahawalpur, Bahawalpur, Pakistan
*(*Corresponding author's e-mail: rukhsana.tabassum@iub.edu.pk)*

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Table S1 DPPH scavenging activity of ZL compounds (ZL11-ZL16)

	%Scavenging of DPPH at different concentrations(µg/mL)					
Compounds	**5**	**10**	**15**	**20**	**25**	**IC_{50} (µg/mL)**
ZL11	53.90	60.3	64.90	70.58	77.05	7.62±0.04
ZL12	46.27	54.11	60.98	70.00	76.07	6.93±0.05
ZL13	44.70	52.54	59.41	67.45	78.43	7.6±0.04
ZL14	40.78	55.09	63.13	70.19	80.39	7.78±0.03
ZL15	47.6	52.94	57.6	62.3	69.6	6.94±0.06
ZL16	47.45	54.31	60.19	65.88	70.19	6.57±0.03
AA*	46.47	52.09	61.52	73.47	77.18	7.066±0.06

*%age scavenging=$((A_0-As/A_0)\times100$ where A_0=Absorbance of blank As=Absorbance of sample
IC_{50}=Concentration of compounds for 50% inhibition of DPPH calculated by non-linear regression
AA*=Ascorbic acid (saturated compound)

Table S2 DPPH scavenging activity of ZL Mn complexes (ZL11Mn-ZL16Mn)

	%Scavenging of DPPH at different concentrations(µg/mL)					
Compounds	**5**	**10**	**15**	**20**	**25**	**IC_{50} (µg/mL)**
ZL11 Mn	48.78	53.41	58.53	65.38	70.97	6.45±0.07
ZL12 Mn	44.14	48.53	52.92	58.29	65.12	11.84±0.01
ZL13 Mn	50.9	55.85	60.73	67.07	71.46	7.09±0.01
ZL14 Mn	42.19	49.02	53.90	59.75	63.65	11.04±0.01
ZL15 Mn	40.24	45.60	50.73	57.00	63.41	11.84±0.04
ZL16 Mn	50.00	56.82	63.90	70.48	75.60	6.629±0.02
AA*	46.47	52.09	61.52	73.47	77.18	7.066±0.06

*%age scavenging=$((A_0-As/A_0)\times100$ where A_0=Absorbance of blank As=Absorbance of sample
IC_{50}=Concentration of compounds for 50% inhibition of DPPH calculated by non-linear regression
AA*=Ascorbic acid (saturated compound)

Table S3 DPPH scavenging activity of ZL Zn complexes (ZL11Zn-ZL16Zn)

	%Scavenging of DPPH at different concentrations(µg/mL)					
Compounds	**5**	**10**	**15**	**20**	**25**	**IC_{50} (µg/mL)**
ZL11 Zn	44.20	49.64	56.73	62.88	70.68	8.31±0.051
ZL12 Zn	48.46	55.55	63.59	68.08	74.46	6.10±0.048
ZL13 Zn	43.49	50.35	56.97	63.59	69.50	8.49±0.046
ZL14 Zn	39.24	47.75	54.60	62.88	72.10	5.65±0.08
ZL15 Zn	43.02	47.99	56.50	63.82	75.41	8.32±0.06
ZL16 Zn	47.28	52.24	57.91	65.48	73.52	7.14±0.075
AA*	46.47	52.09	61.52	73.47	77.18	7.066±0.06

*%age scavenging=$((A_0\text{-}As/A_0)\times100$ where A_0=Absorbance of blank As=Absorbance of sample
IC_{50}=Concentration of compounds for 50% inhibition of DPPH calculated by non-linear regression
AA*=Ascorbic acid (saturated compound)

Table S4 NO scavenging activity of (ZL11-ZL16)

	%Scavenging of NO at different concentrations(µg/mL)					
Compounds	**5**	**10**	**15**	**20**	**25**	**IC_{50} (µg/mL)**
ZL11	47.39	55.72	67.70	75.52	89.06	6.46±0.046
ZL12	48.43	56.25	66.14	83.85	92.18	6.38±0.095
ZL13	47.91	59.37	68.27	73.95	81.25	5.89±0.038
ZL14	45.31	54.16	64.58	74.47	85.93	7.015±0.068
ZL15	44.79	59.37	71.87	82.81	92.18	6.47±0.052
ZL16	41.28	45.69	51.21	57.61	65.34	11.2±0.053
AA*	48.79	56.83	60,21	66.21	70.50	6.79±0.026

*%age scavenging=$((A_0\text{-}As/A_0)\times100$ where A_0=Absorbance of blank As=Absorbance of sample
IC_{50}=Concentration of compounds for 50% inhibition of NO calculated by non-linear regression
AA*=Ascorbic acid (saturated compound)

Table S5 NO scavenging activity of ZL Mn complexes (ZL11Mn-ZL16Mn)

Compounds	%Scavenging activity of NO at different concentrations(µg/mL)					IC_{50} (µg/mL)
	5	10	15	20	25	
ZL11 Mn	51.17	58.63	64.39	70.78	77.61	7.29±0.021
ZL12 Mn	51.81	56.71	62.02	68.23	75.69	5.99±0.060
ZL13 Mn	57.56	64.17	64.81	75.22	82.30	6.56±0.07
ZL14 Mn	52.66	59.06	64.17	72.49	78.03	6.98±0.024
ZL15 Mn	58.84	65.24	71.21	78.03	82.67	6.35±0.096
ZL16 Mn	46.26	53.09	60.55	66.52	74.41	7.10±0.67
AA*	48.79	56.83	60,21	66.21	70.50	6.79±0.026

*%age scavenging=((A_0-As/A_0)×100 where A_0=Absorbance of blank As=Absorbance of sample
IC_{50}=Concentration of compounds for 50% inhibition of NO calculated by non-linear regression
AA*=Ascorbic acid (saturated compound)

Table S6 NO scavenging activity of ZL Zn complexes (ZL11Zn-ZL16Zn)

	%Scavenging of NO at different concentrations(µg/mL)					
Compounds	**5**	**10**	**15**	**20**	**25**	**IC_{50} (µg/mL)**
ZL11 Zn	52.75	65.51	64.13	73.79	82.75	7.32±0.044
ZL12 Zn	40.00	50.65	59.65	68.31	80.34	6.77±0.078
ZL13 Zn	56.89	64.13	76.89	95.17	96.55	6.63±0.034
ZL14 Zn	49.65	56.20	68.96	83.10	92.41	6.073±0.09
ZL15 Zn	57.58	61.72	66.53	72.06	74.13	6.59±0.06
ZL16 Zn	38.37	44.56	51.48	59.48	68.01	6.3±0.065
AA*	48.79	56.83	60,21	66.21	70.50	6.79±0.026

*%age scavenging=((A_0-As/A_0)×100 where A_0=Absorbance of blank As=Absorbance of sample
IC_{50}=Concentration of compounds for 50% inhibition of NO calculated by non-linear regression
AA*=Ascorbic acid (saturated compound)

Table S7 XRD results of ZL16

2θ	θ	d-spacing	FWHM	L (nm)	Average crystal size
10.74636	5.37318	8.225984823	1.18314	6.982190712	4.092028
11.54993	5.774965	7.655415376	1.10716	7.532510562	
12.29678	6.14839	7.192087335	1.21595	6.863252946	
22.94915	11.474575	3.872156537	1.22748	6.897537714	
24.94915	12.474575	3.56609868	23.04805	0.368707523	

Table S8 XRD results of ZL16Mn

2θ	θ	d-spacing	FWHM	L (nm)	Average crystal size
17.27887	8.639435	5.127954552	1.74161	4.710136115	4.341198
26.69156	13.34578	3.337127729	1.84368	4.625347197	
31.54908	15.77454	2.83352031	2.04612	4.213871061	
34.75143	17.375715	2.579391656	1.69112	5.141034797	
38.69814	19.34907	2.324924593	1.55375	5.659906526	
55.70464	27.85232	1.648779008	1.55422	6.038090462	

Table S9 XRD results of ZL16Zn

2θ	θ	d-spacing	FWHM	L (nm)	Average crystal size
14.56013	7.280065	6.078780792	15.82403	0.520125408	1.573858
36.06904	18.03452	2.488129959	1.6689	5.22864124	
56.82144	28.41072	1.618995715	1.83956	5.128155248	
58.82144	29.41072	1.568625859	131.56428	0.072397477	
61.30325	30.651625	1.510935026	142.4885	0.067689174	

Table S10 Thermo analytical results (TG and DTG) of ligand (ZL14) and Metal complex

Compound	**TG Range(°C)**	**DTG max Range(°C)**	**Estimated Calculated %** **Mass Loss Total Mass**		**Assignment**	**Metallic Residue**
(ZL14).H_2O	20-190 190-400 400-800	112, 305, 535, 595	3.17 20.39 11.18 14.69	(3.93) (20.61) (10.02) (14.42)	Loss of H_2O Loss of C_4H_7ClLoss of CO_2 Loss of C_3H_8	$C_4H_7ClN_2O$
Mn(ZL14).$3H_2O$	20-100 100-190 190-488 488-880	113, 168, 534, 581	2.11 2.51 1.31 12.87	(3.71) (3.91) (1.78) (12.72)	Loss of $2H_2O$ Loss of HCl Loss of CH_4 Loss of C_8H_{16}	$C_{33}H_6ClN_2$ MnO
Zn (ZL14).$3H_2O$	31-101 101-400 550-600	165, 292, 373, 463	2.18 1.14 3.18 3.99	(3.68) (1.70) (4.76) (3.40)	Loss of $2H_2O$ Loss of CH_4 Loss of CO_2 Loss of C_2H_6	$C_{41}H_{81}Cl_2N_2$ ZnO

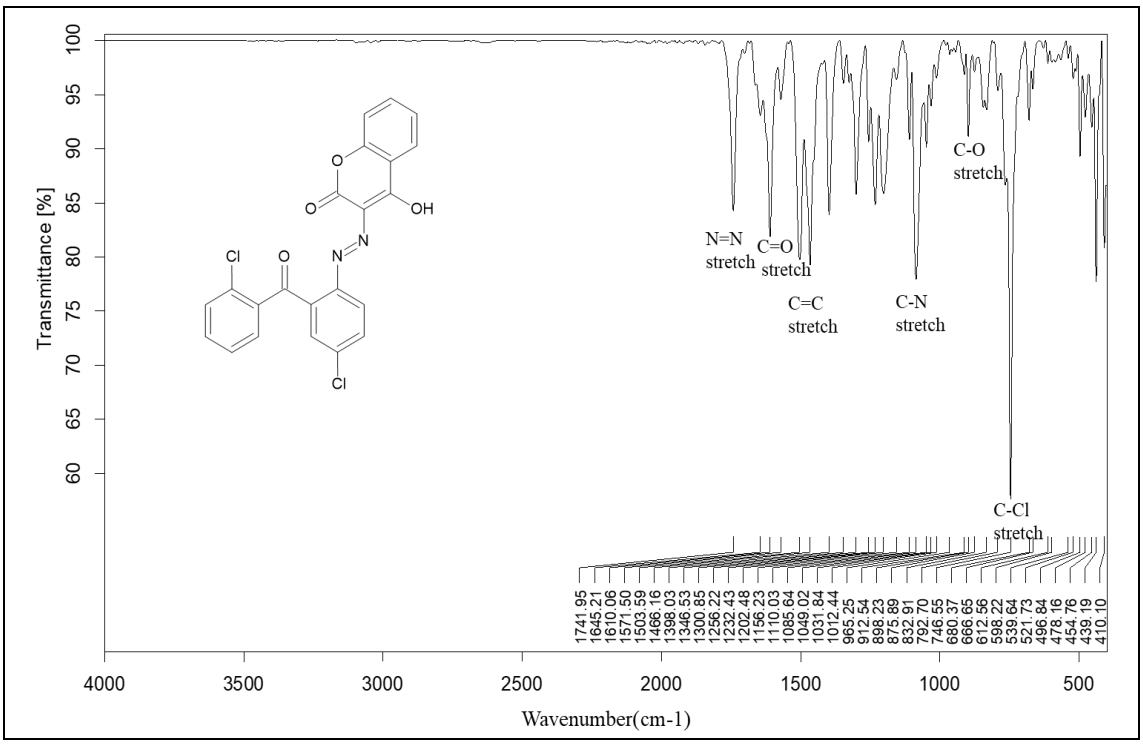

Figure S1. FTIR spectrum of ZL11

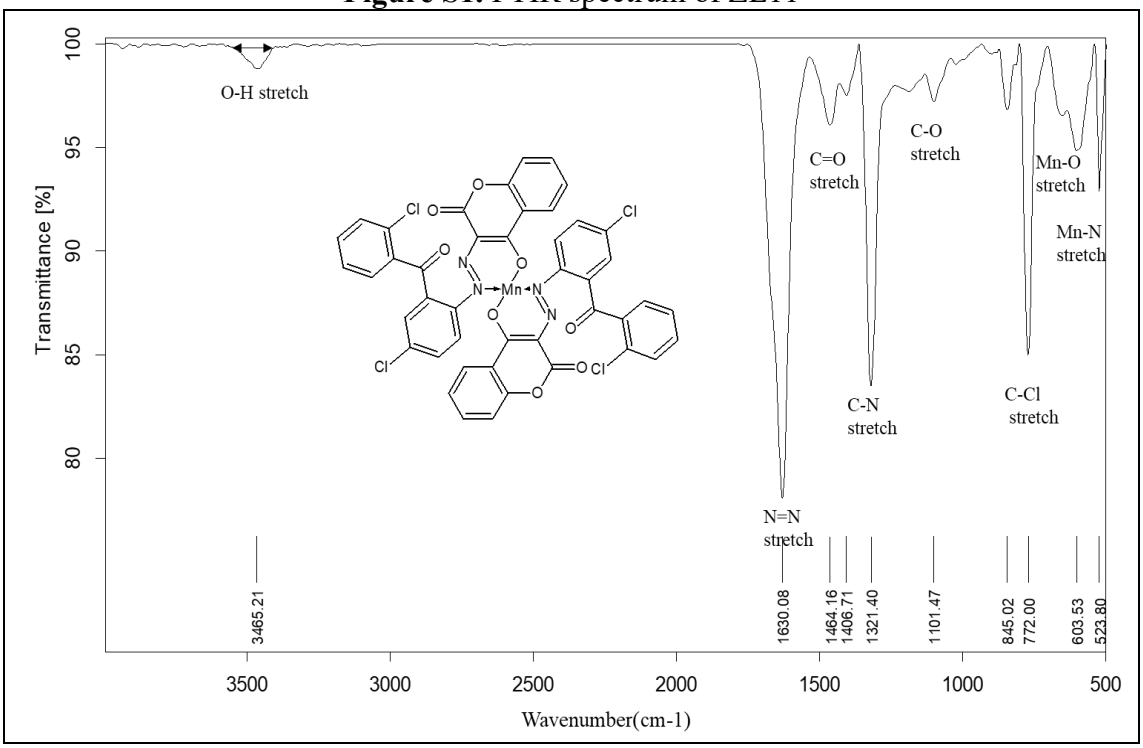

Figure S2. FTIR spectrum of ZL11 Mn

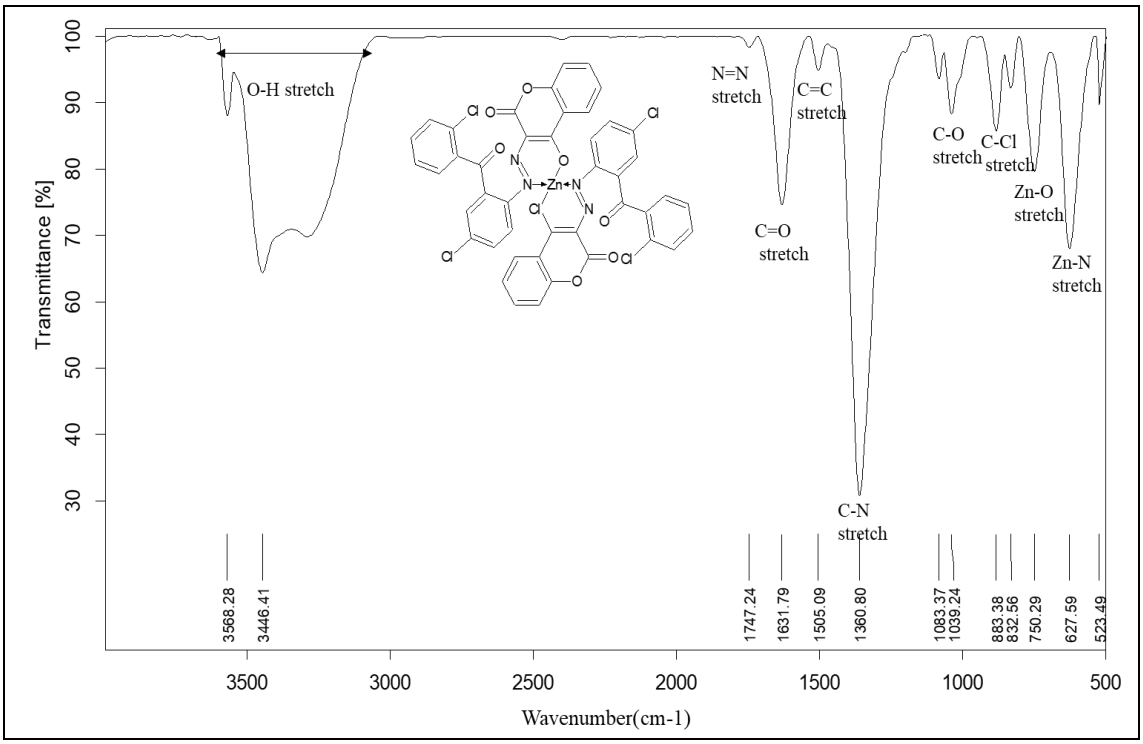

Figure S3. FTIR spectrum of ZL11 Zn

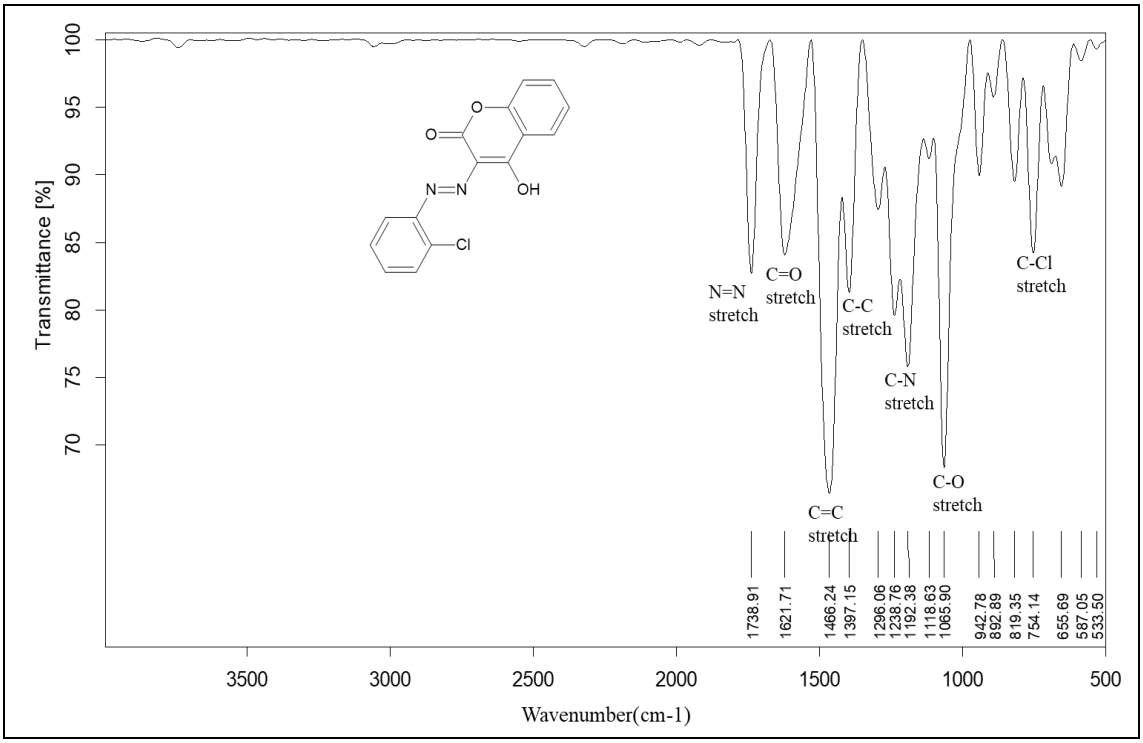

Figure S4. FTIR spectrum of ZL12

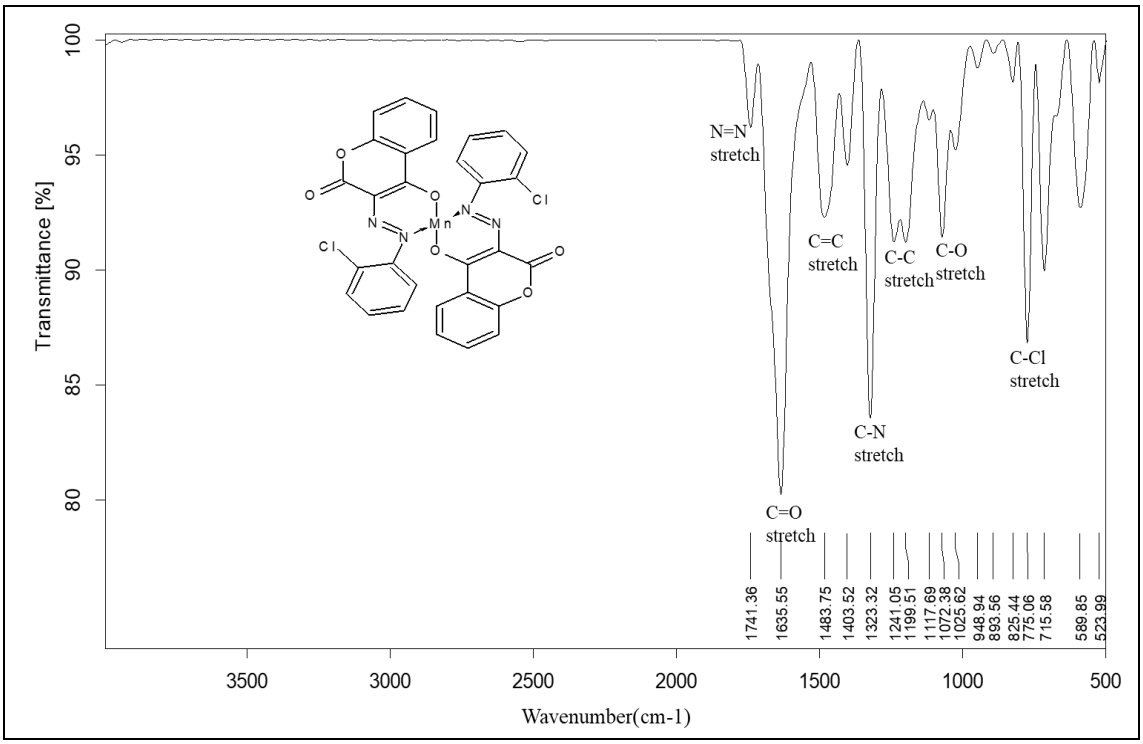

Figure S5. FTIR spectrum of ZL12Mn

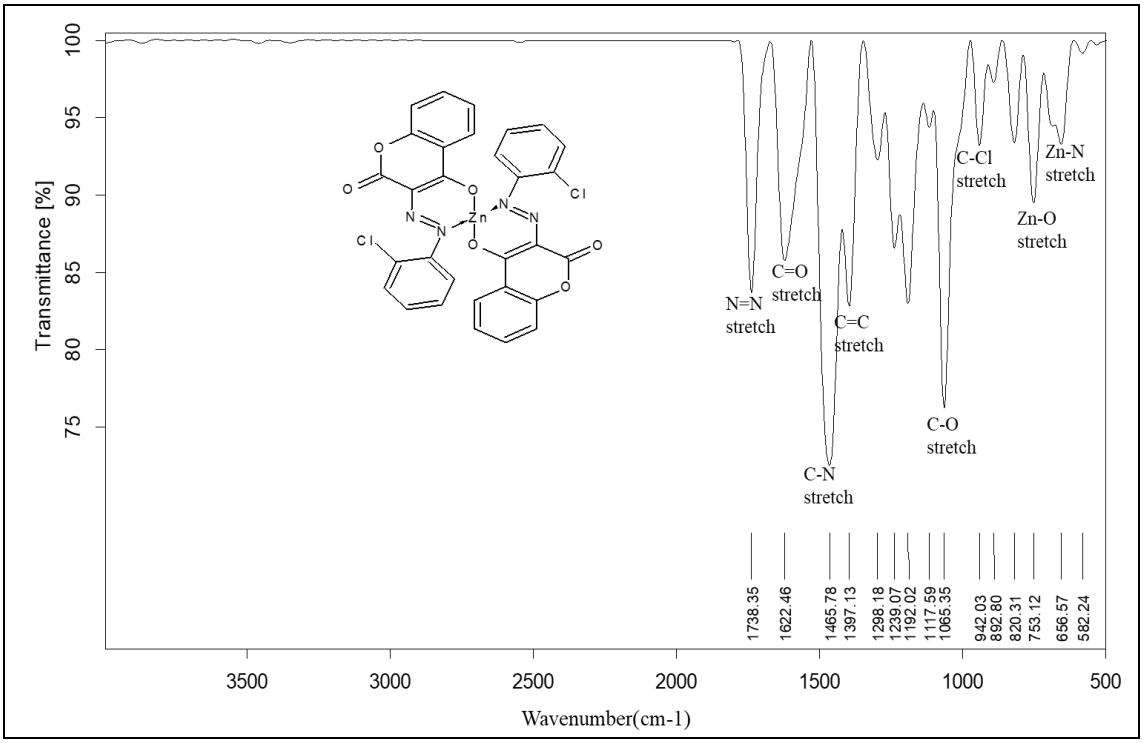

Figure S6. FTIR spectrum of ZL12Zn

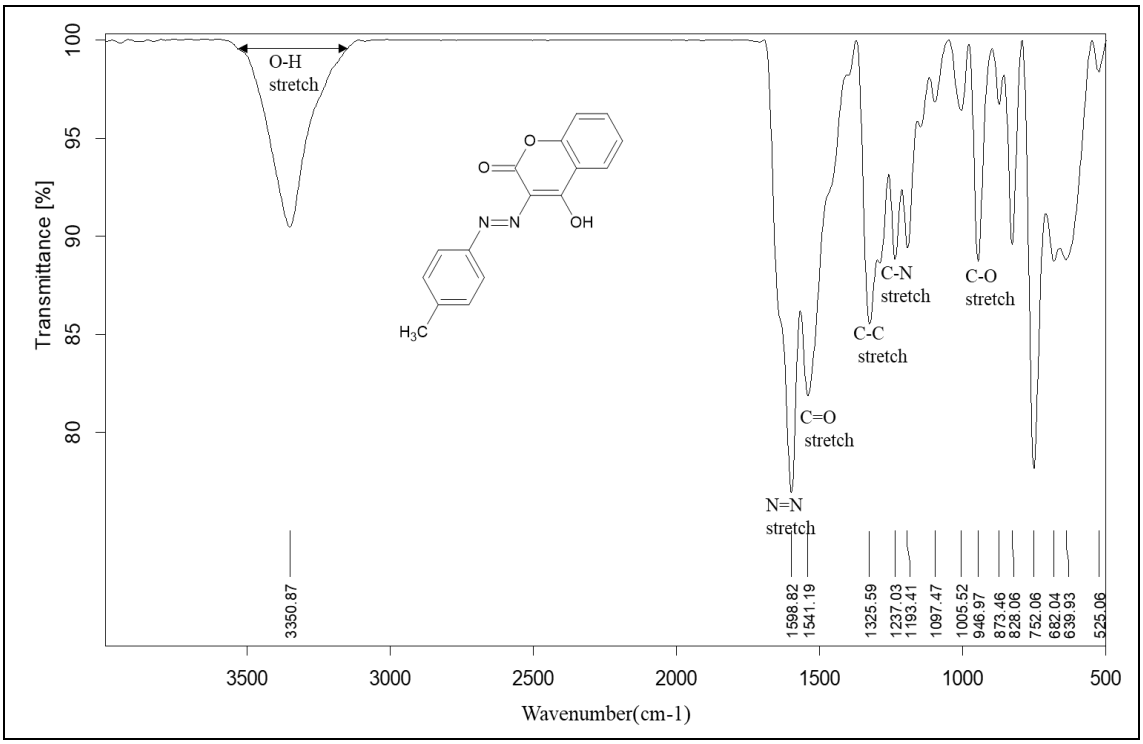

Figure S7. FTIR spectrum of ZL13

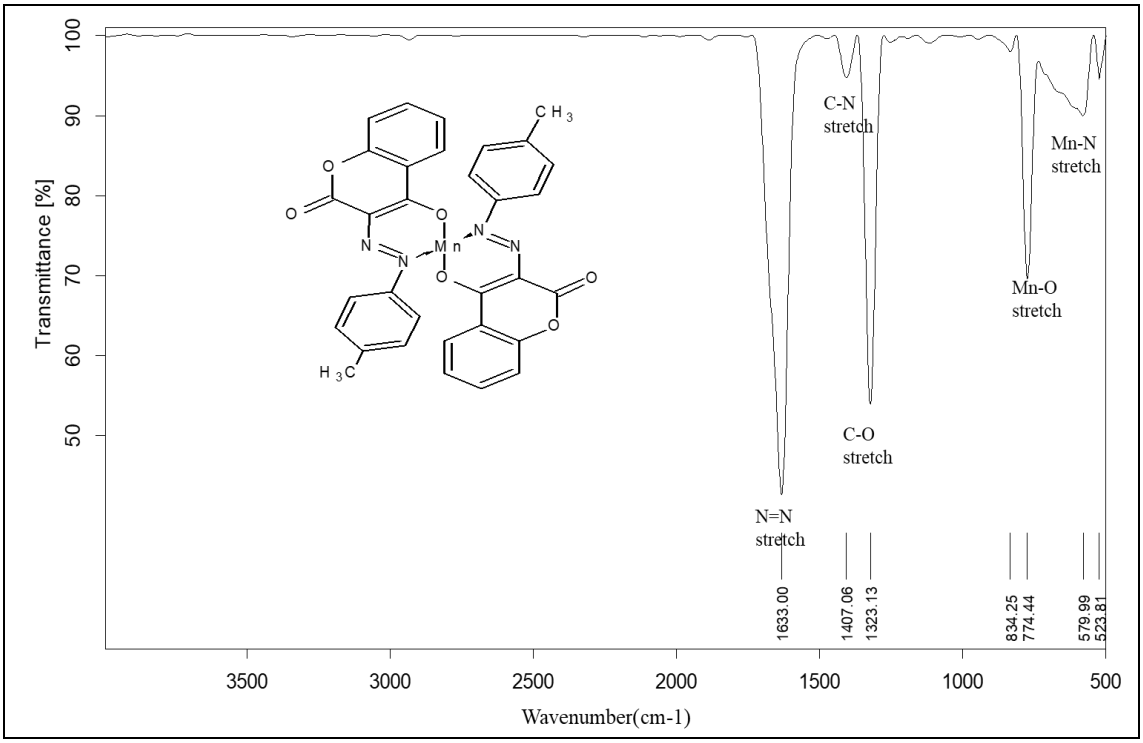

Figure S8. FTIR spectrum of ZL13Mn

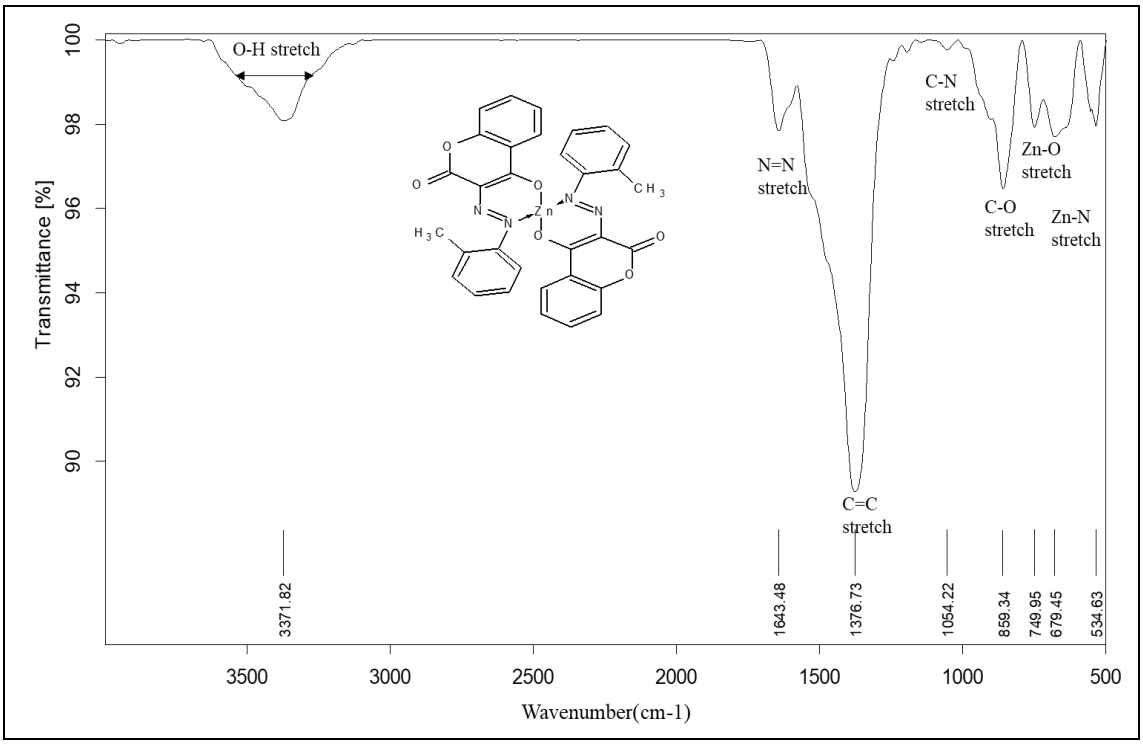

Figure S9. FTIR spectrum of ZL13 Zn

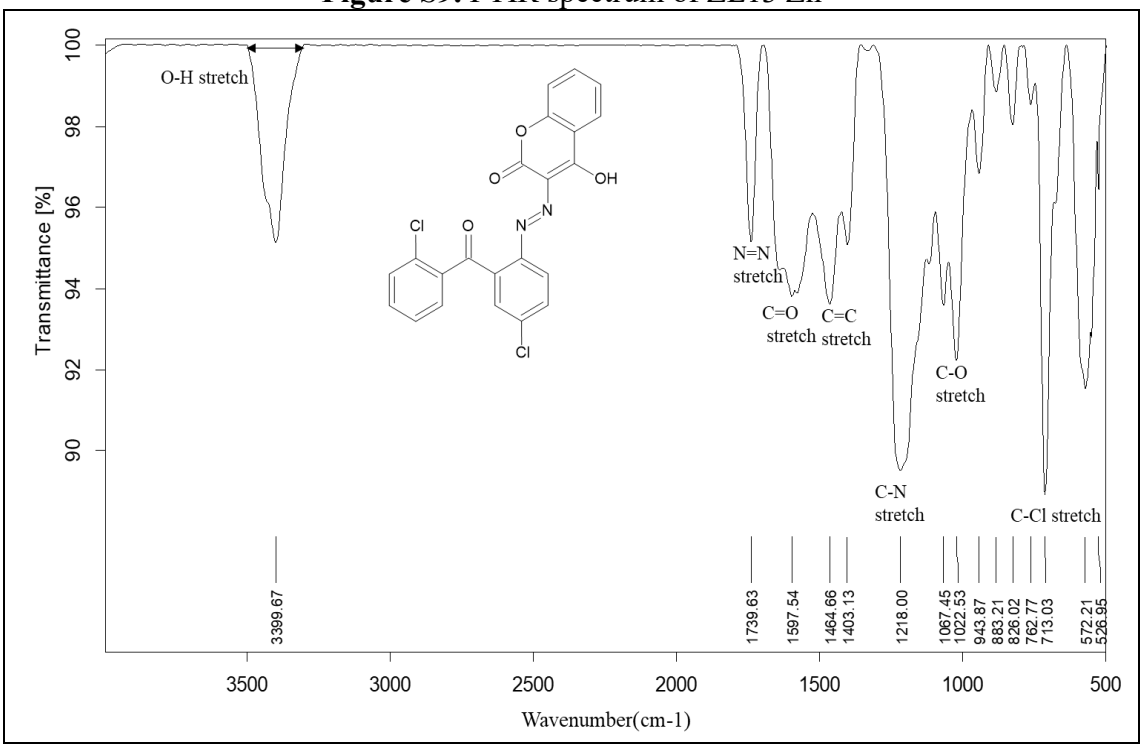

Figure S10. FTIR spectrum of ZL14

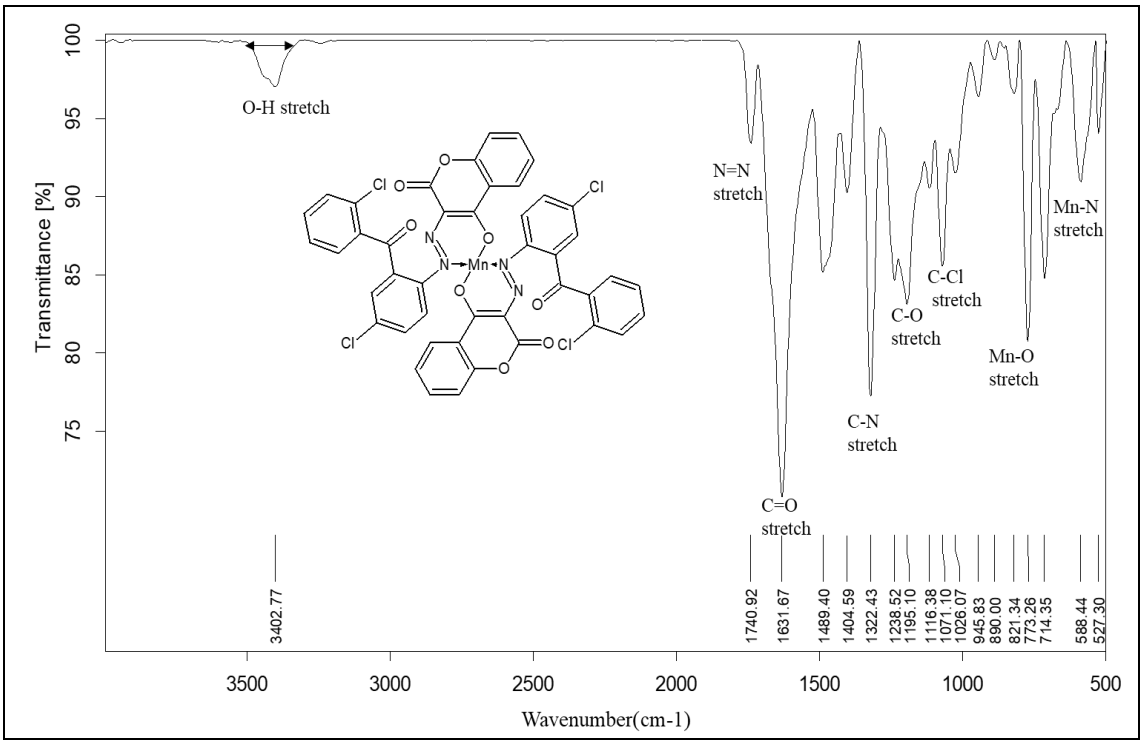

Figure S11. FTIR spectrum of ZL14Mn

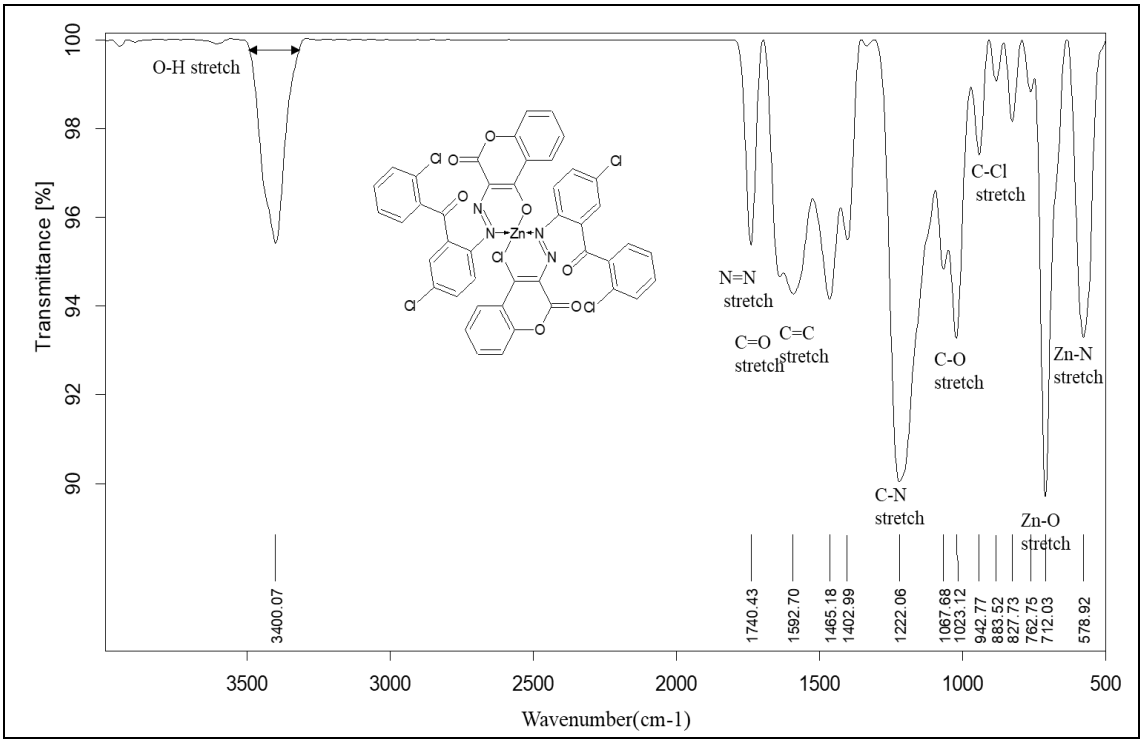

Figure S12. FTIR spectrum of ZL14 Zn

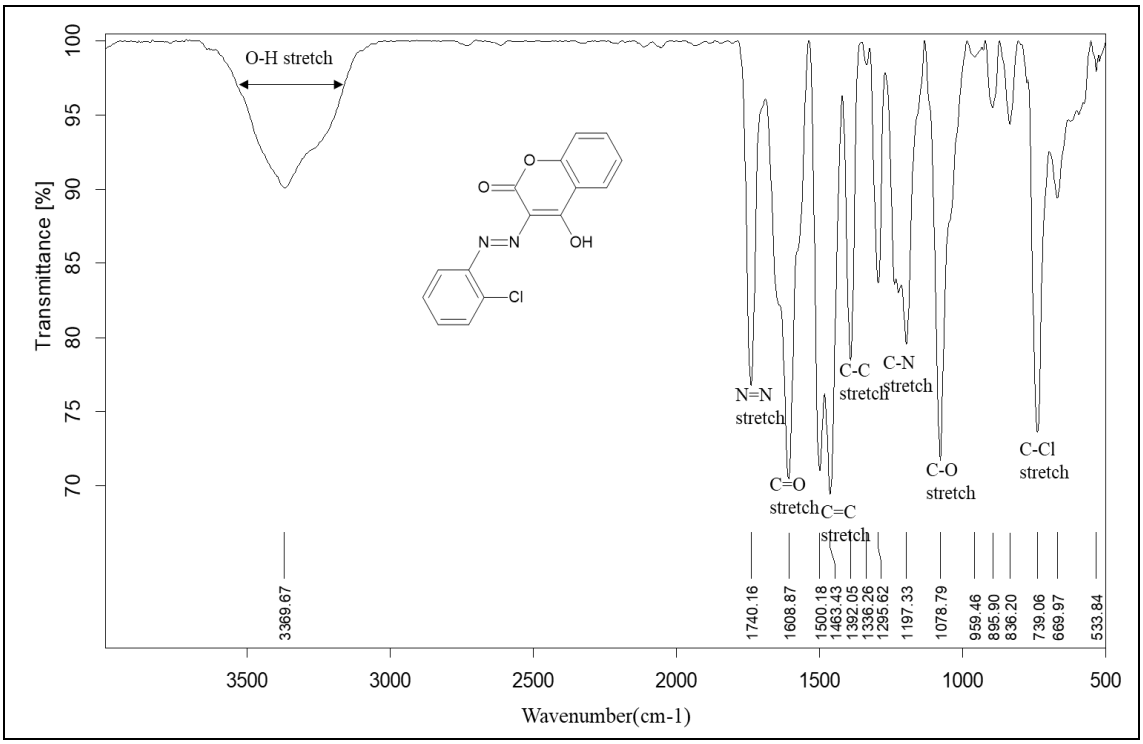

Figure S13. FTIR spectrum of ZL15

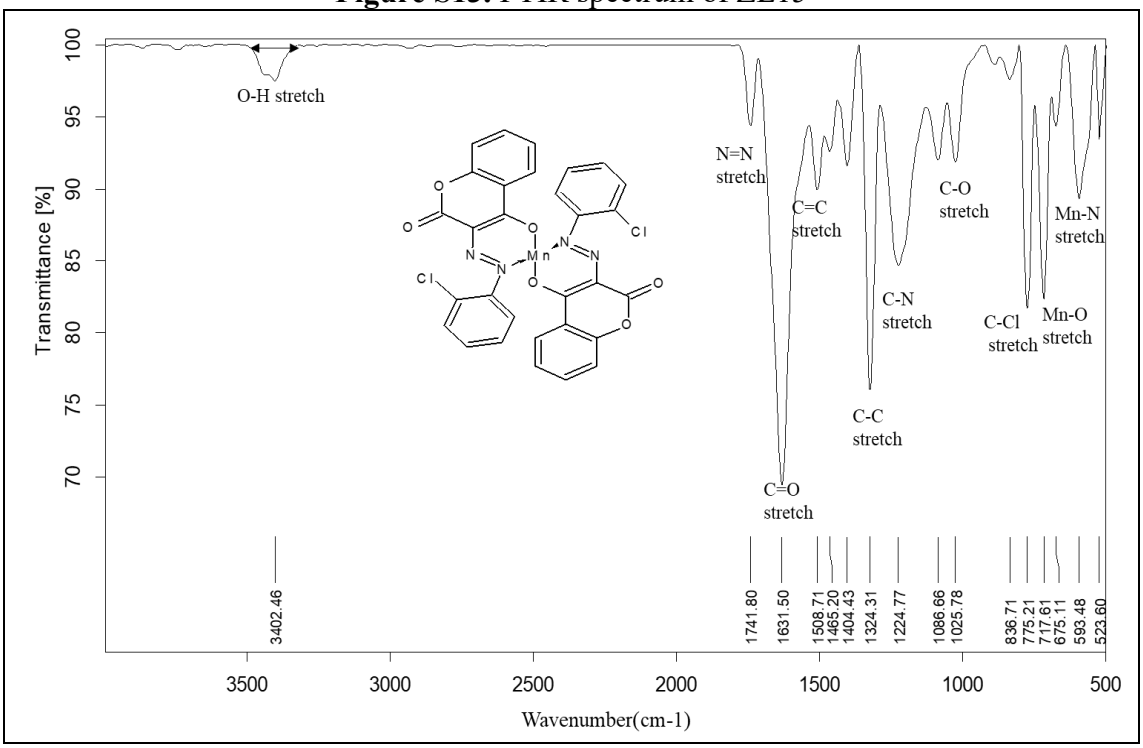

Figure S14. FTIR spectrum of ZL15Mn

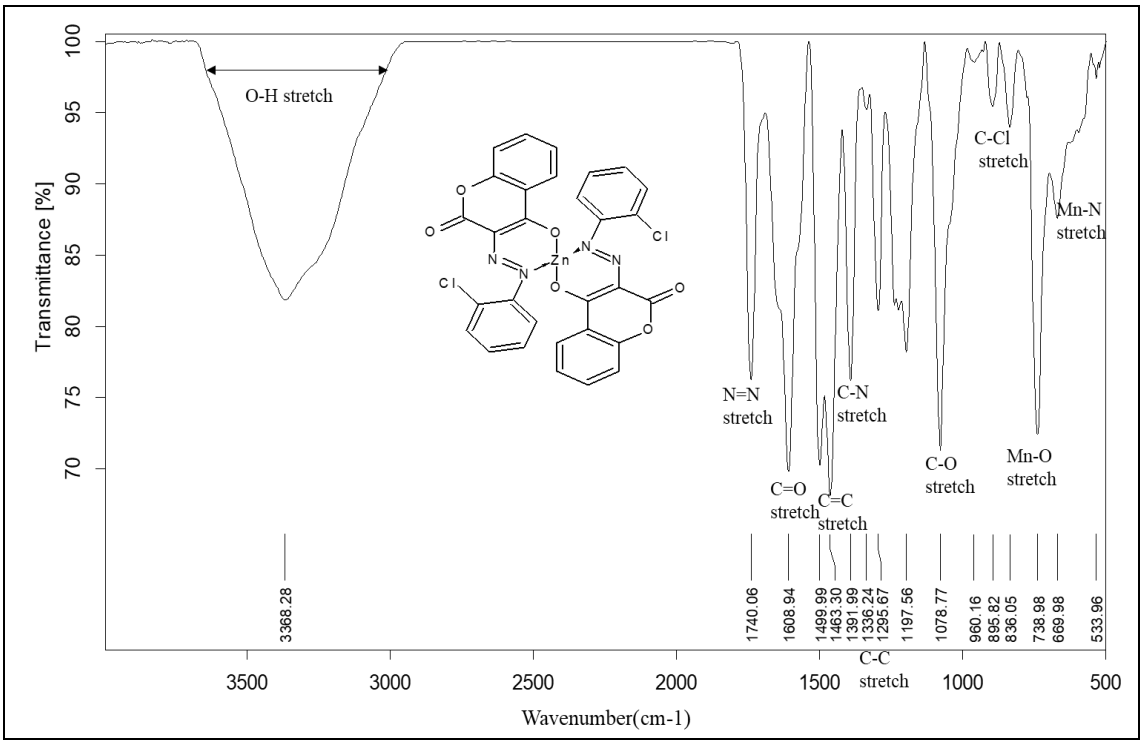

Figure S15. FTIR spectrum of ZL15 Zn

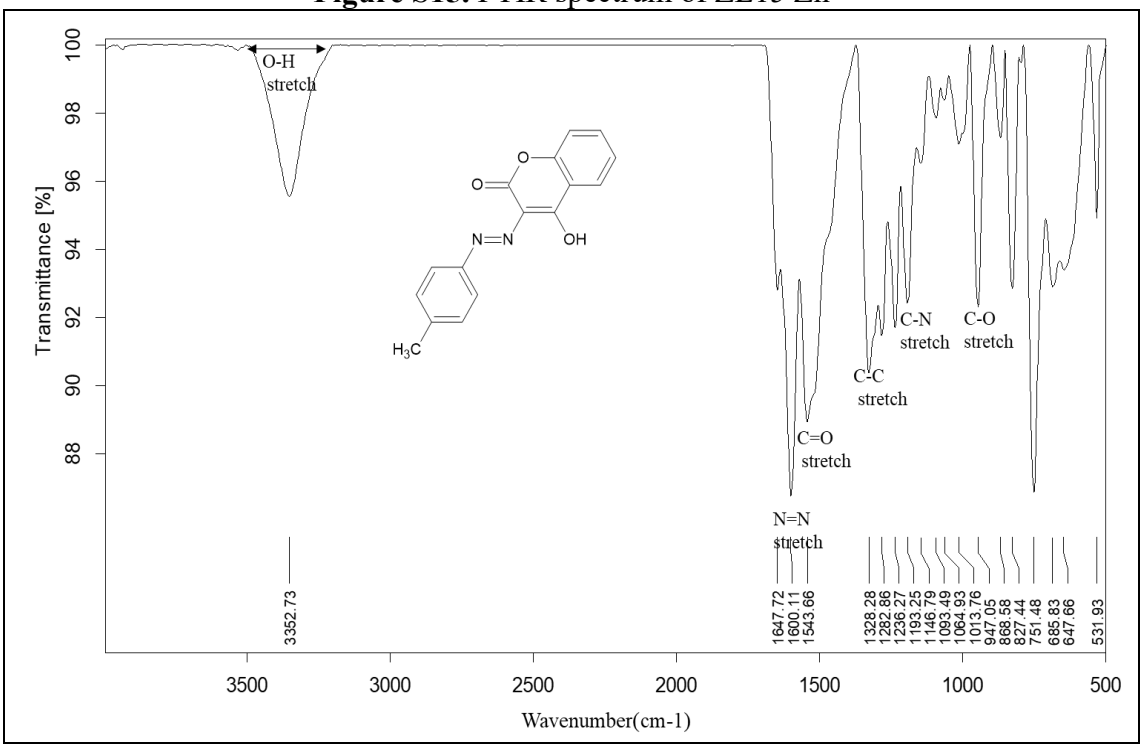

Figure S16. FTIR spectrum of ZL16

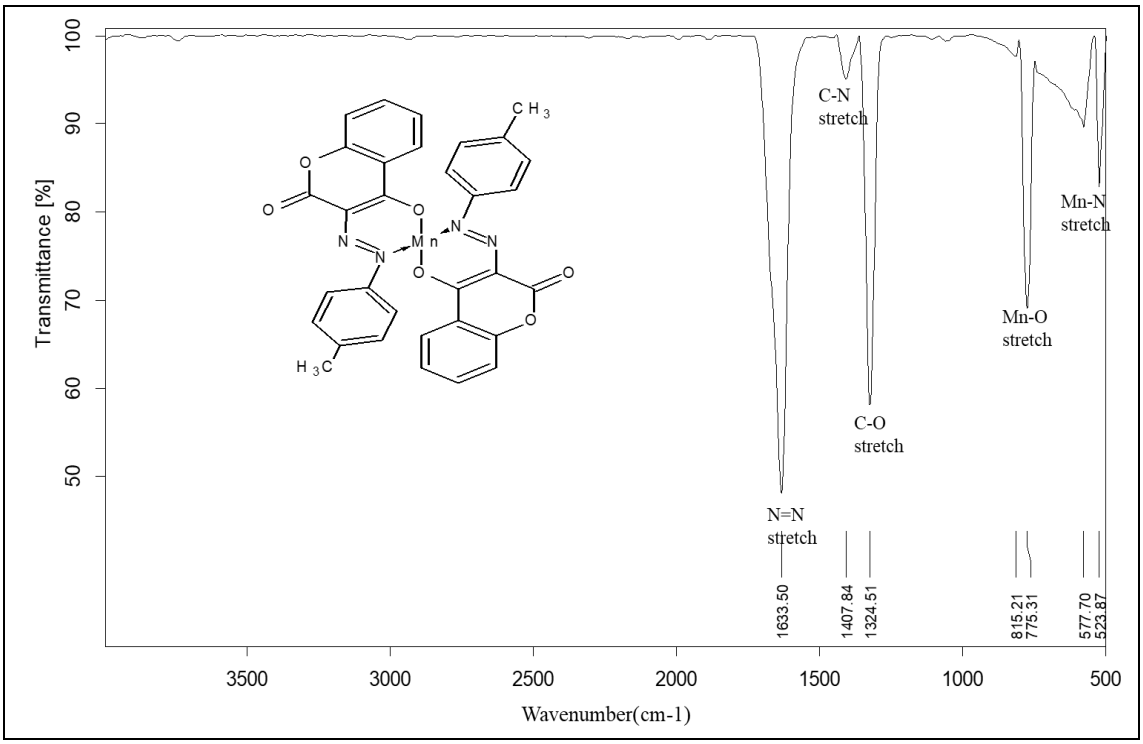

Figure S17. FTIR spectrum of ZL16Mn

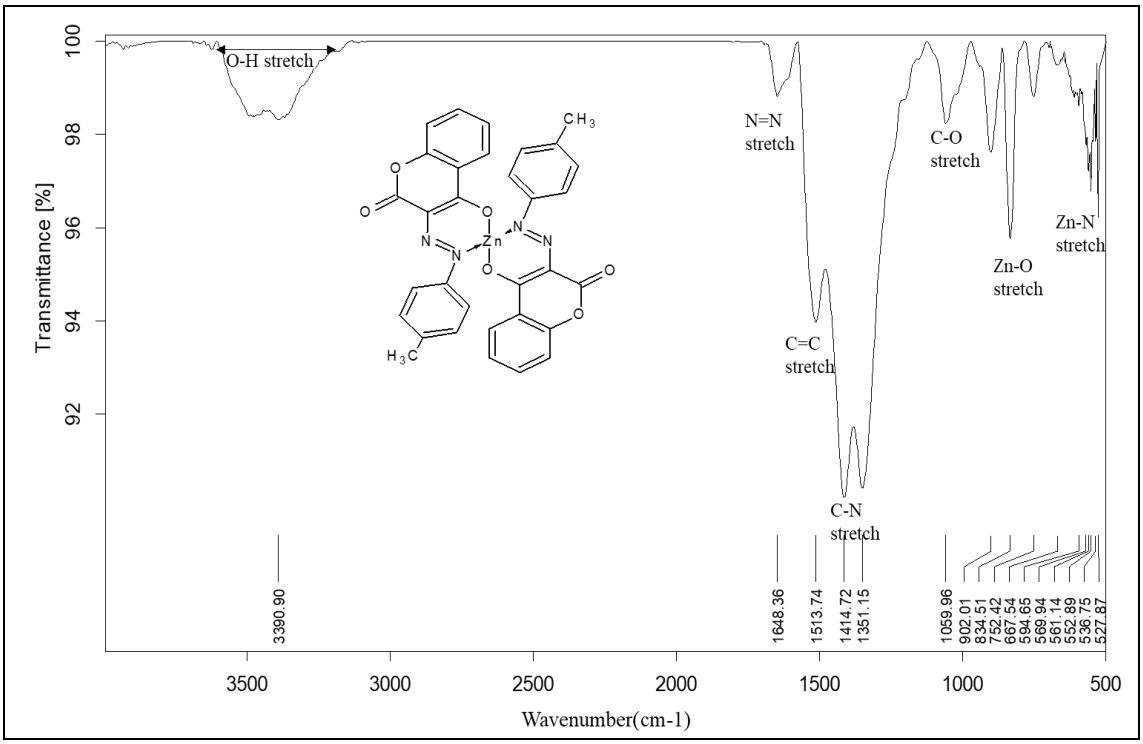

Figure S18. FTIR spectrum of ZL16 Zn

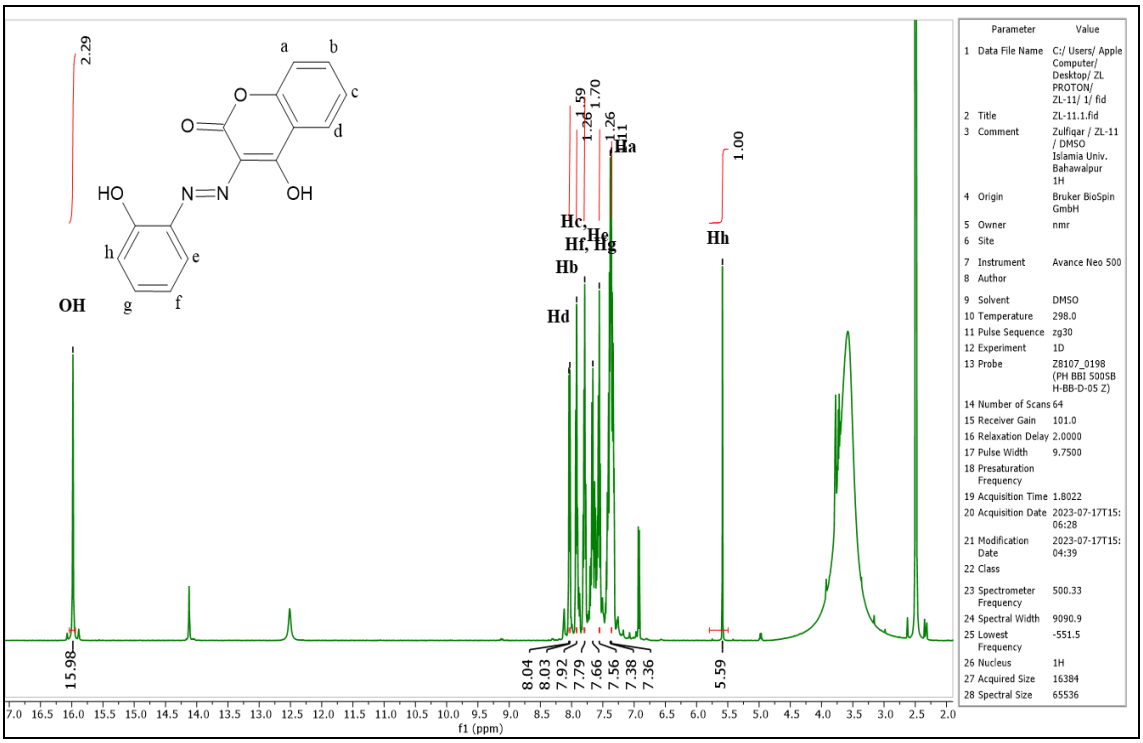

Figure S19. ^{1}HNMR spectrum of ZL11

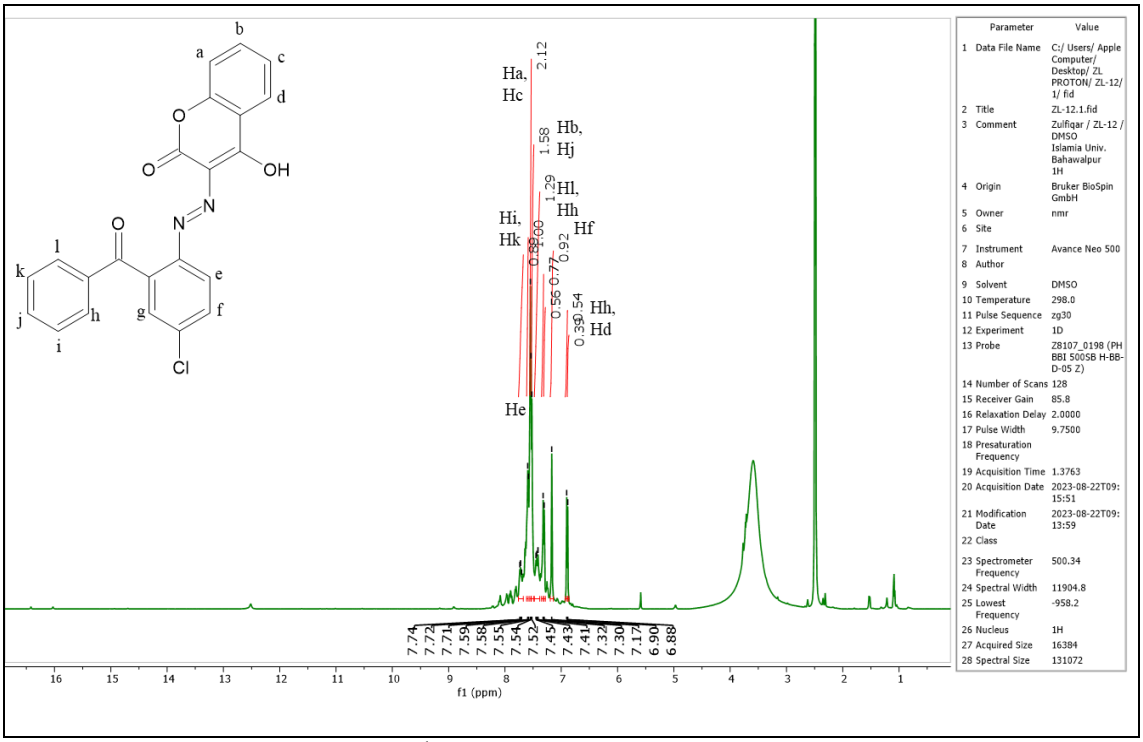

Figure S20. ^{1}HNMR spectrum of ZL12

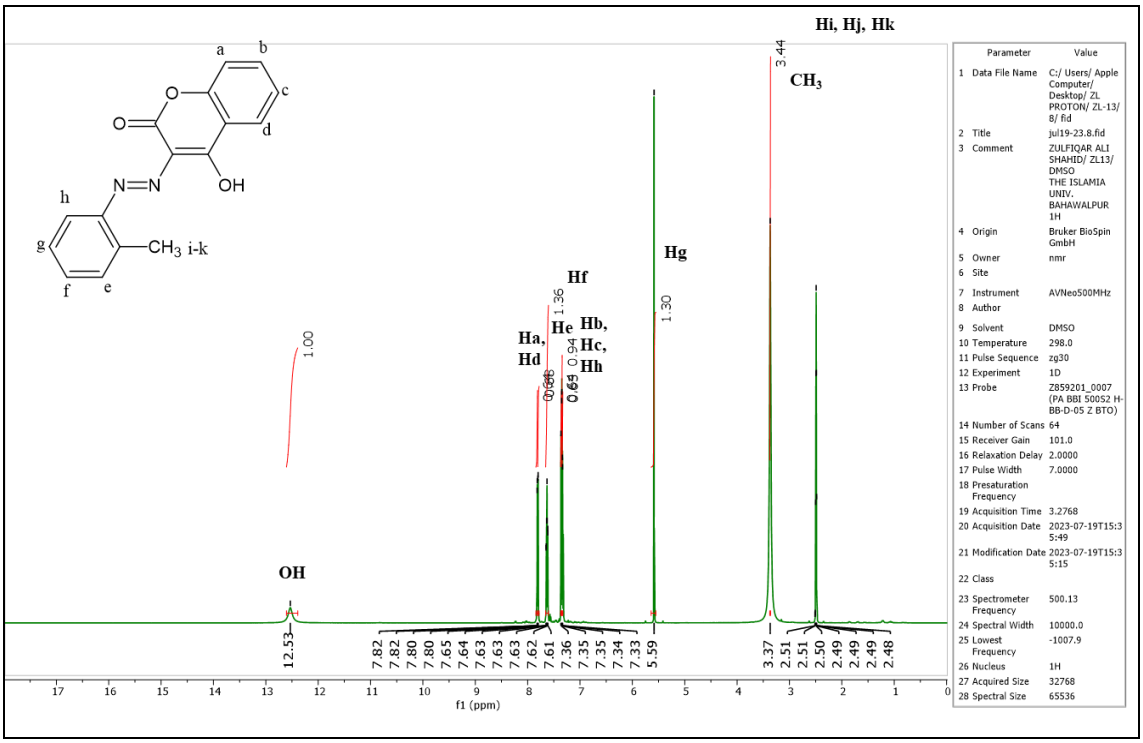

Figure S21. [1]HNMR spectrum of ZL13

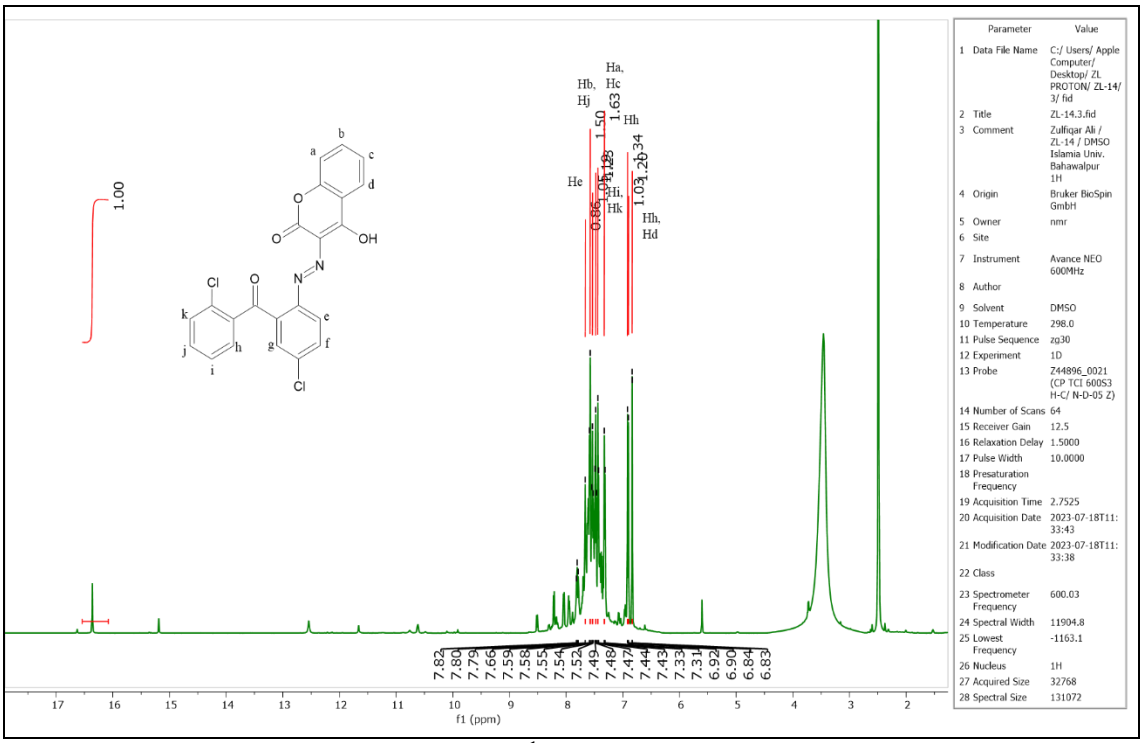

Figure S22. [1]HNMR spectrum of ZL14

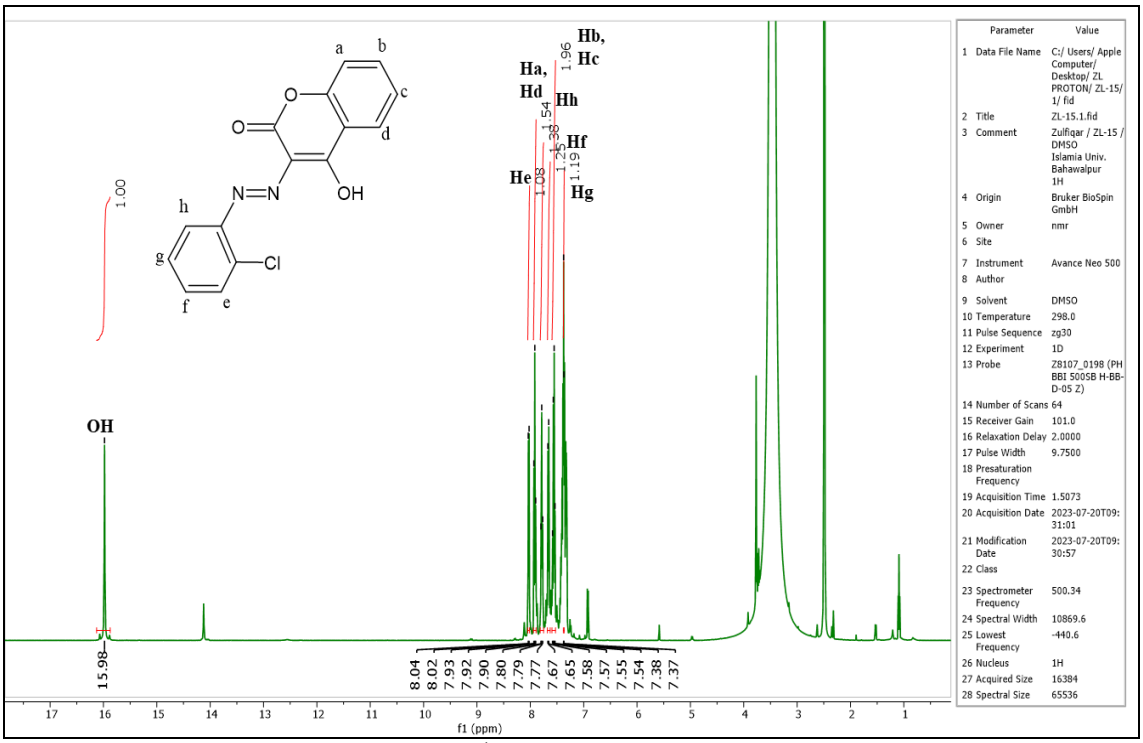

Figure S23. [1]HNMR spectrum of ZL15

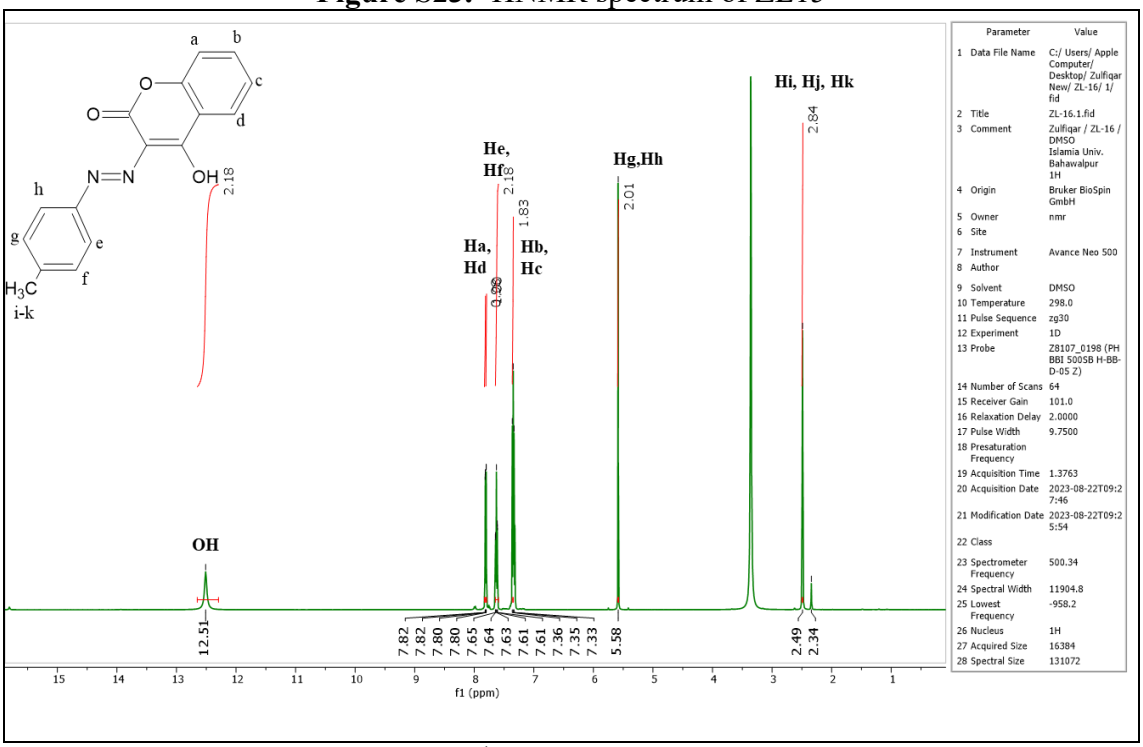

Figure S24. [1]HNMR spectrum of ZL16

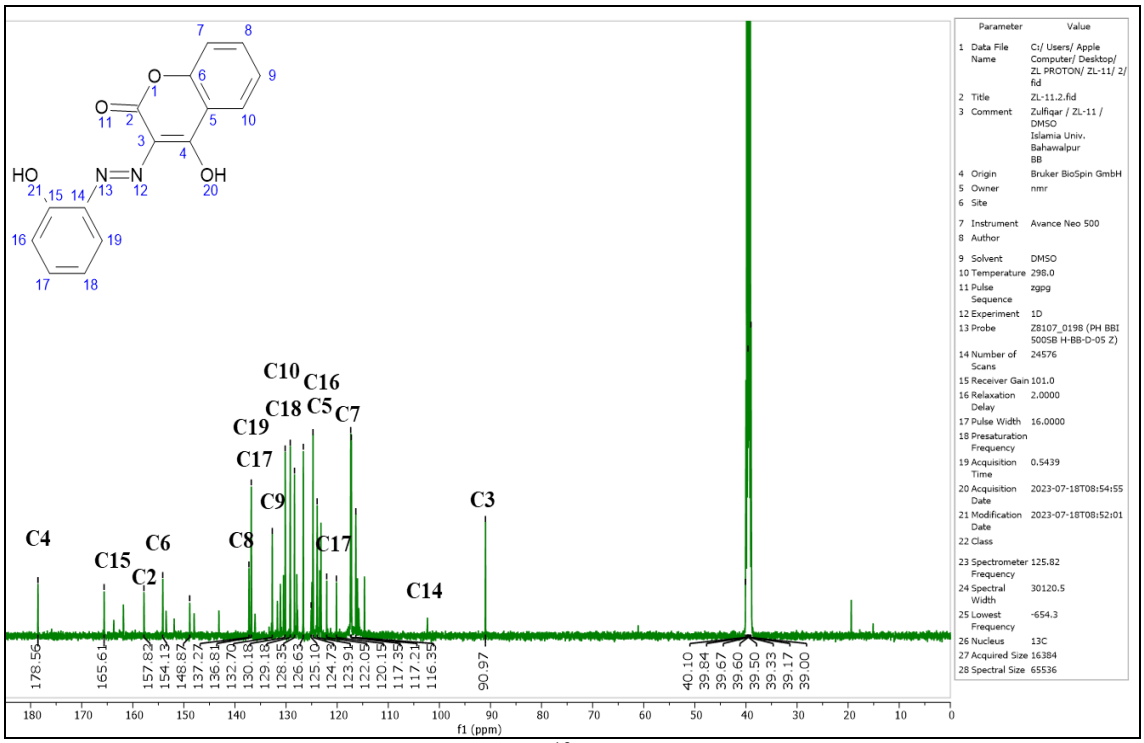

Figure S25. ^{13}CNMR spectrum of ZL11

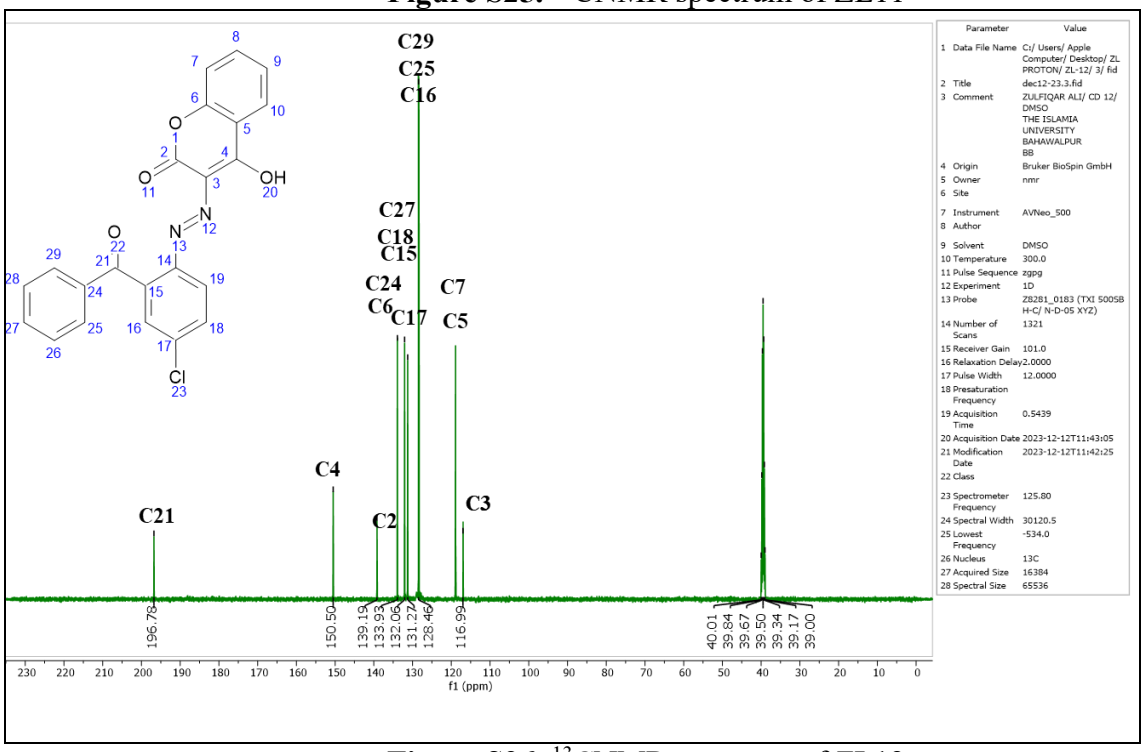

Figure S26. ^{13}CNMR spectrum of ZL12

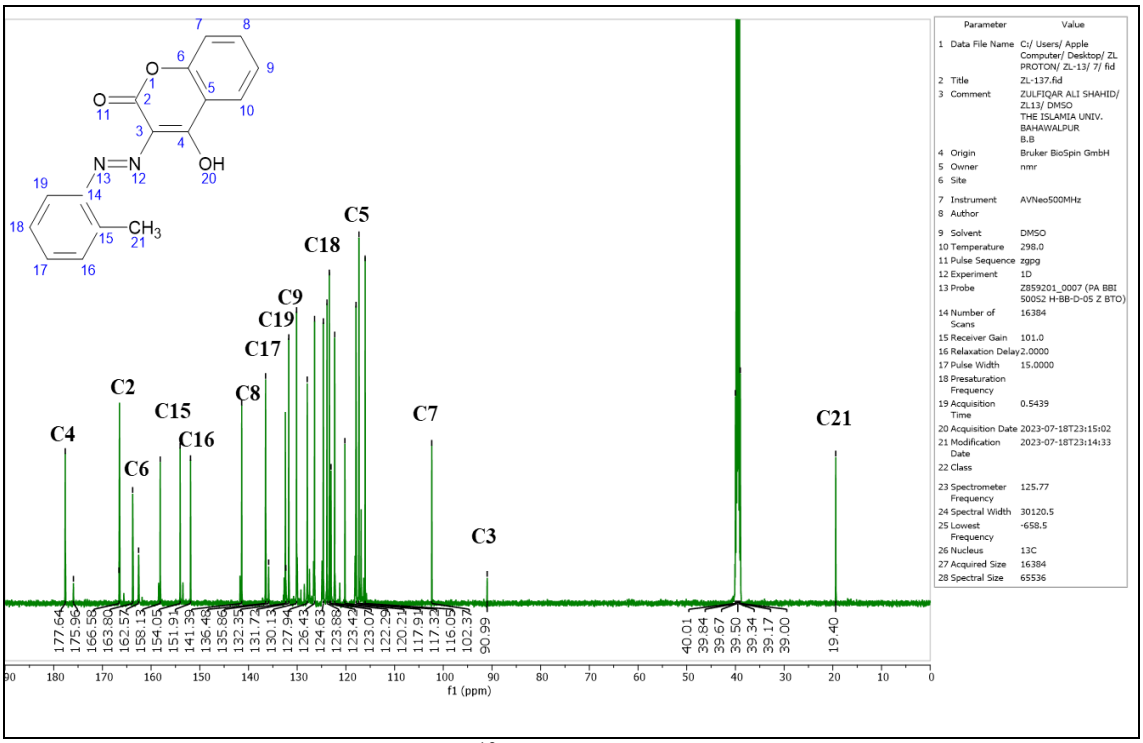

Figure S27. ^{13}CNMR spectrum of ZL13

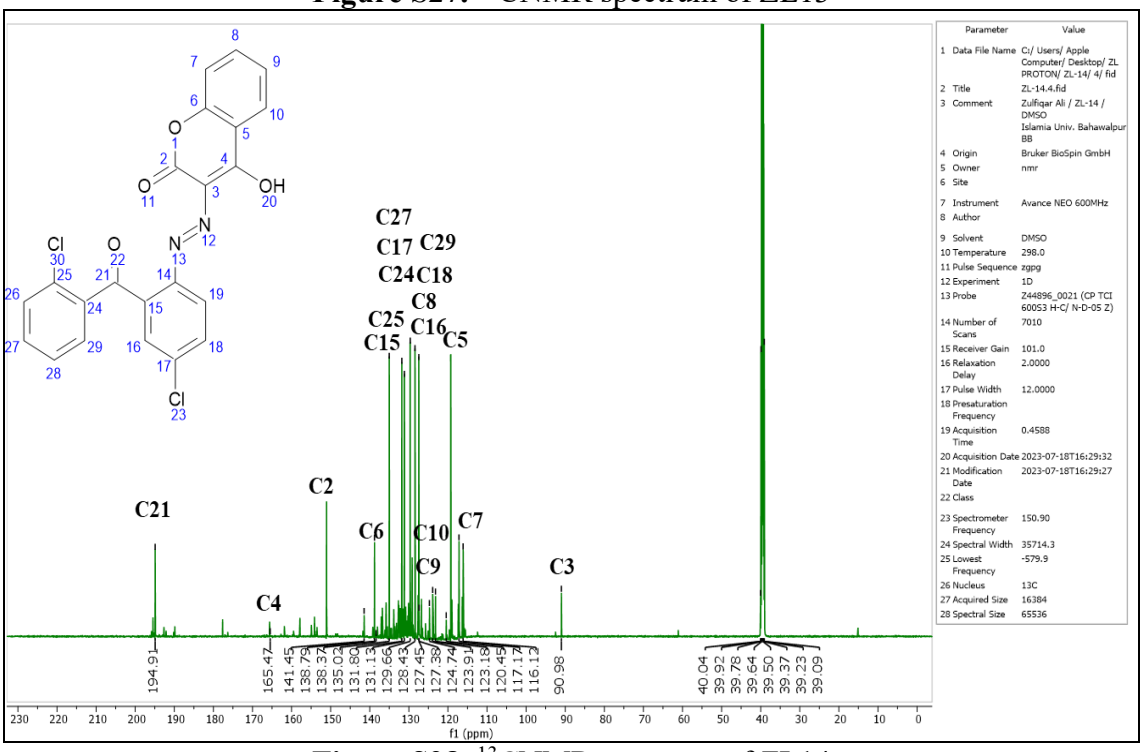

Figure S28. ^{13}CNMR spectrum of ZL14

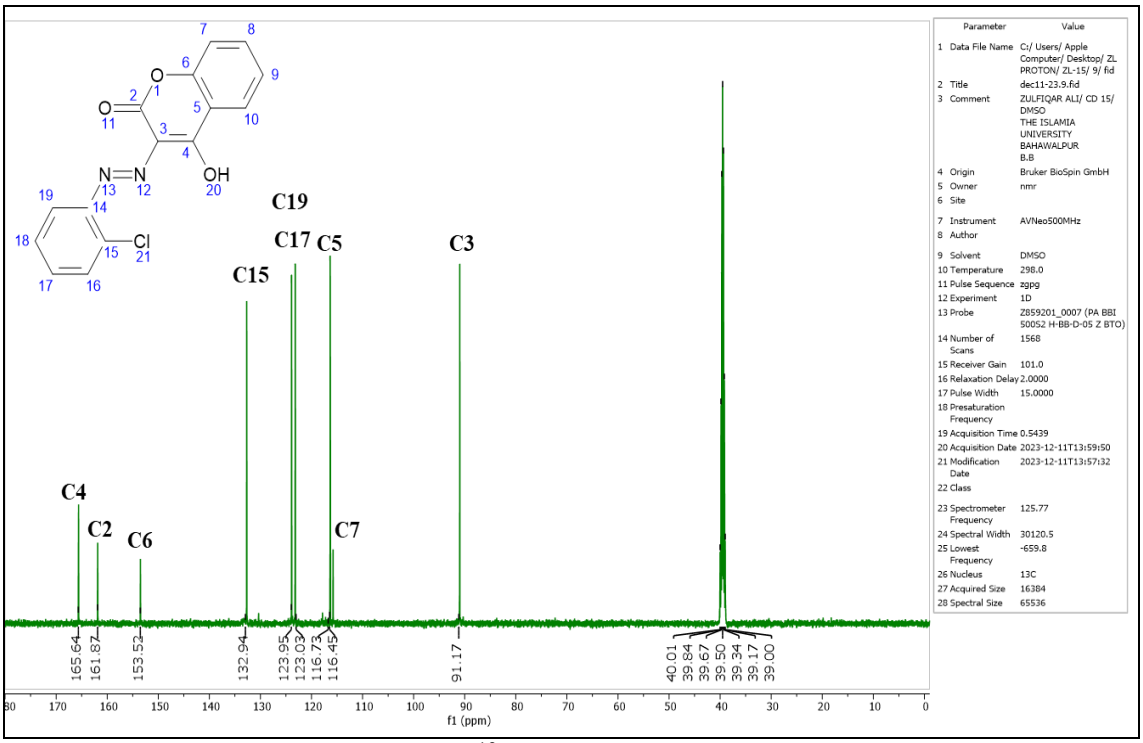

Figure S29. ^{13}CNMR spectrum of ZL15

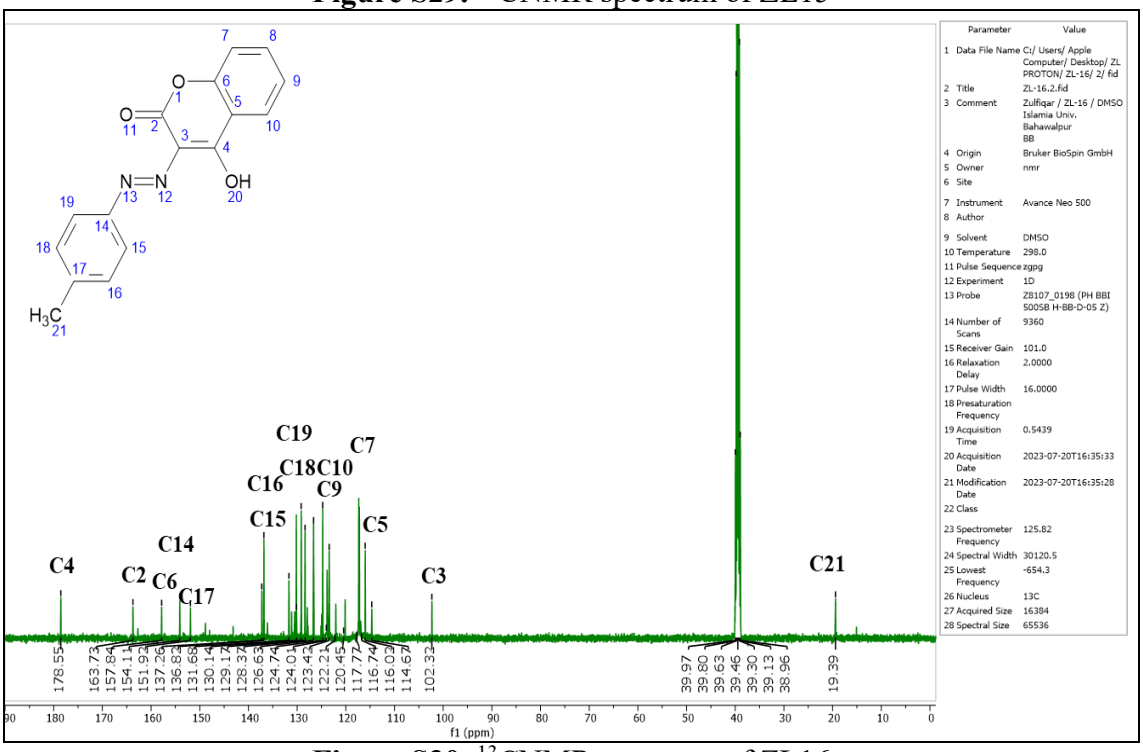

Figure S30. ^{13}CNMR spectrum of ZL16

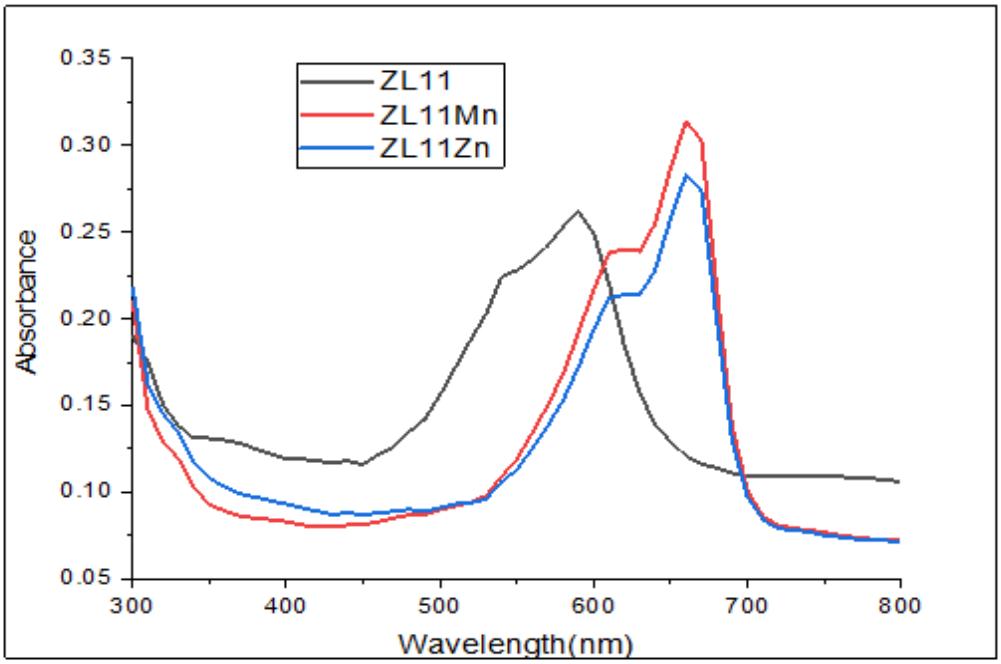

Figure S31. UV-VIS spectrum of ZL11, ZL11Mn, ZL11Zn

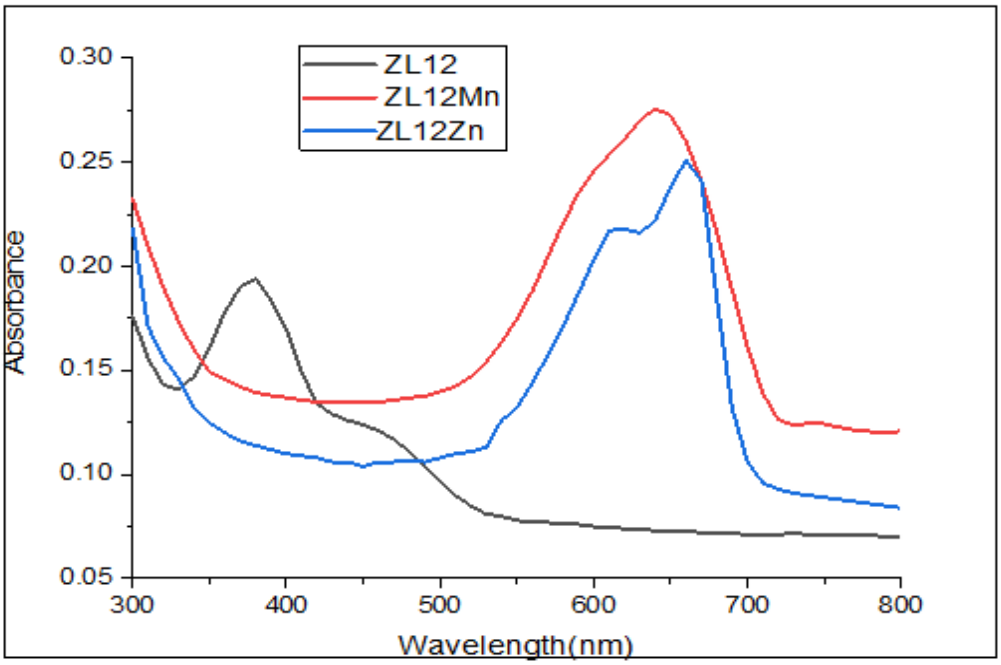

Figure S32. UV-VIS spectrum of ZL12, ZL12Mn, ZL12Zn

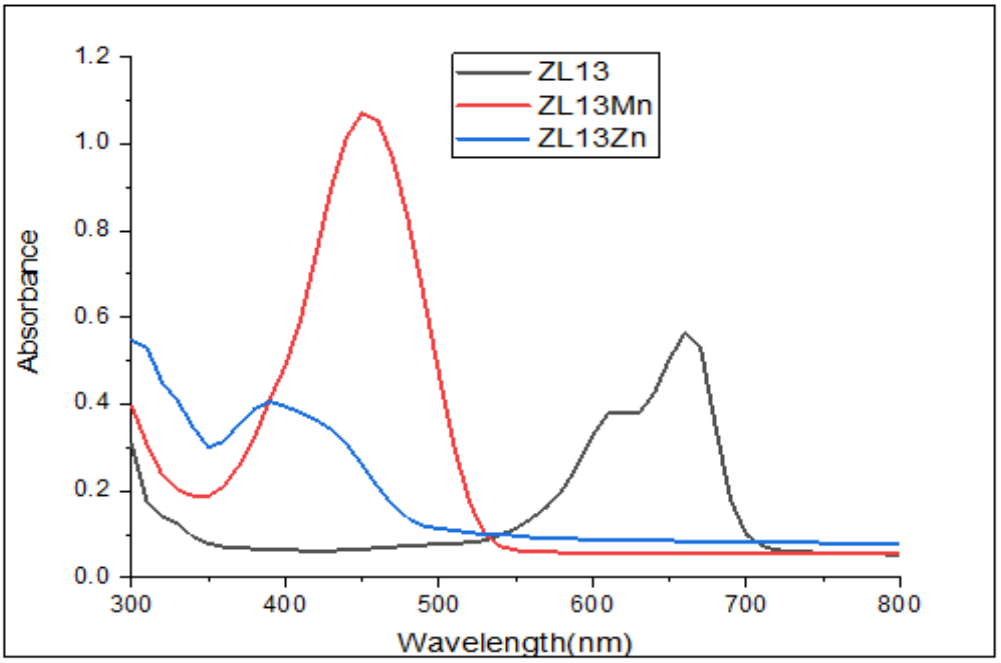

Figure.S33. UV-VIS spectrum of ZL13, ZL13Mn, ZL13Zn

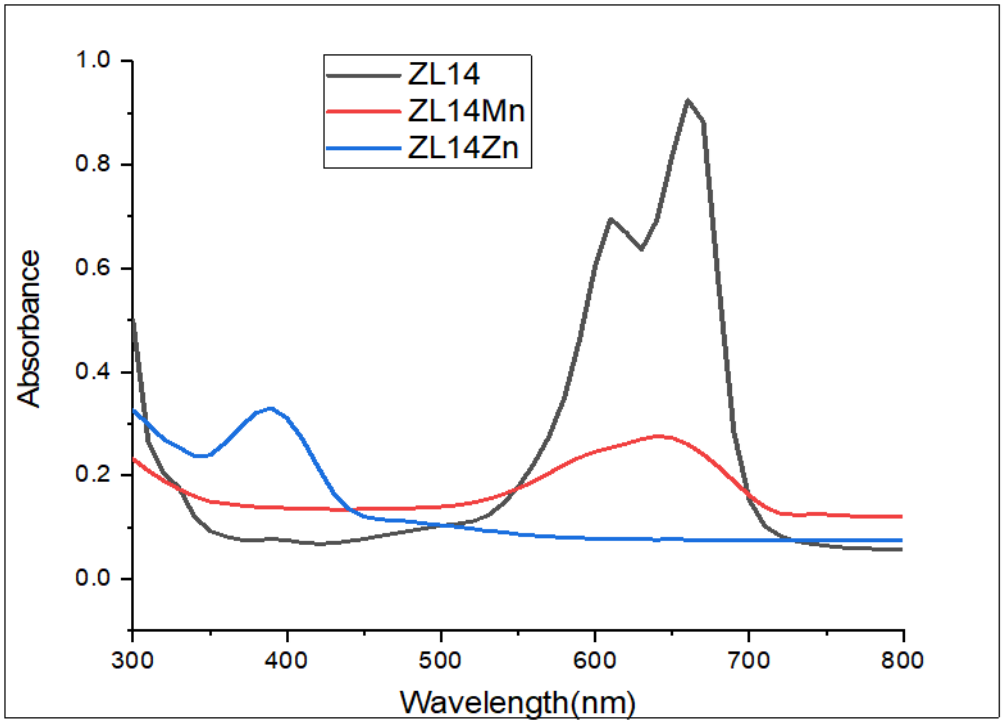

Figure S34. UV-VIS spectrum of ZL14, ZL14Mn, ZL14Zn

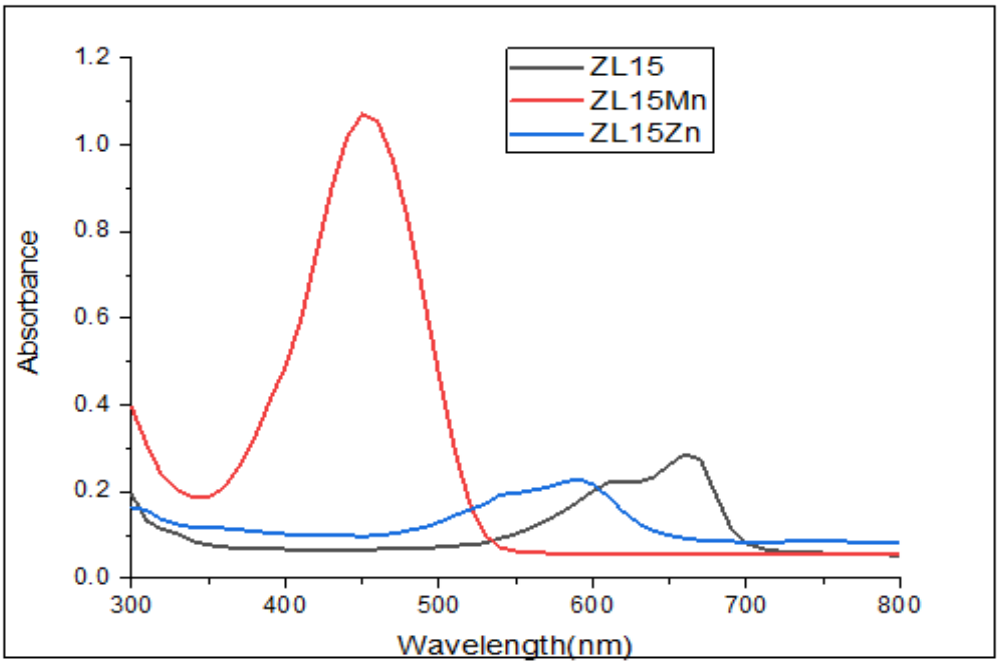

Figure S35. UV-VIS spectrum of ZL15, ZL15Mn, ZL15Zn

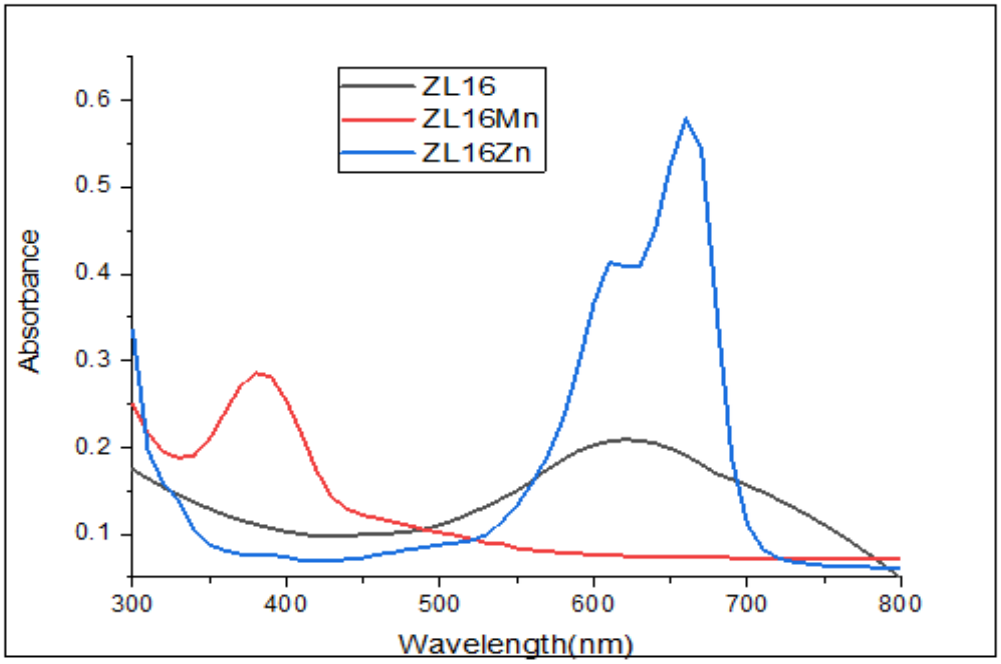

Figure S36. UV-VIS spectrum of ZL16, ZL16Mn, ZL16Zn

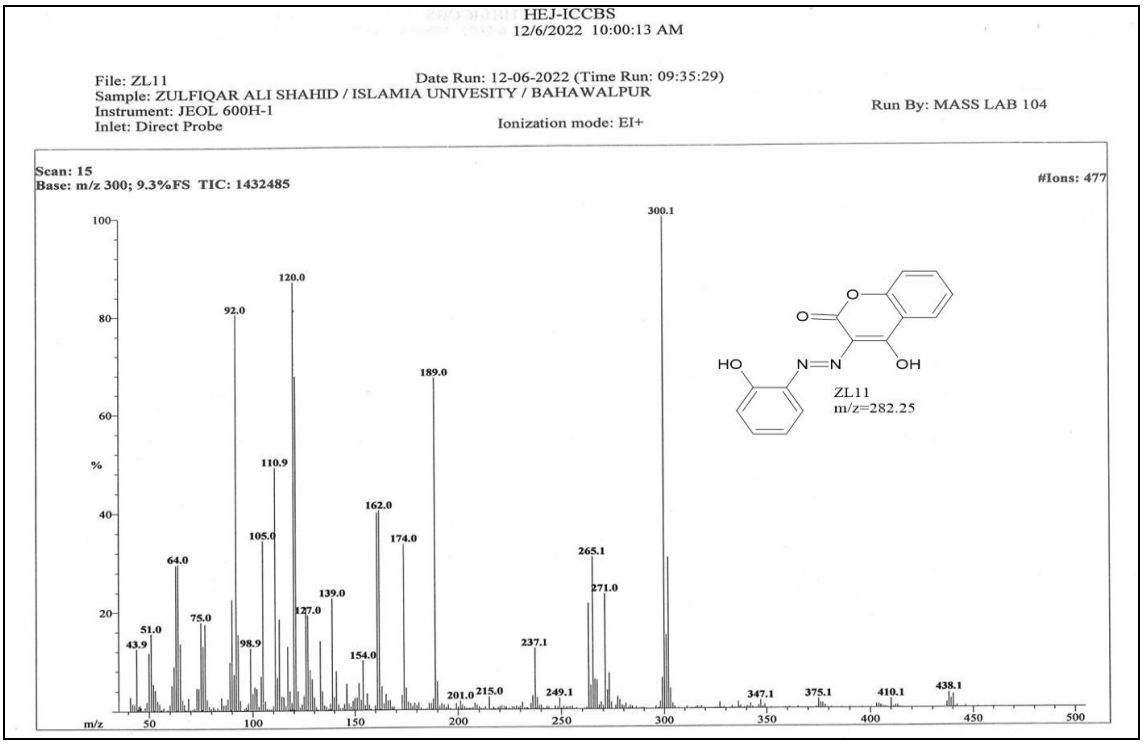

Figure S37. Mass spectrum of ZL11

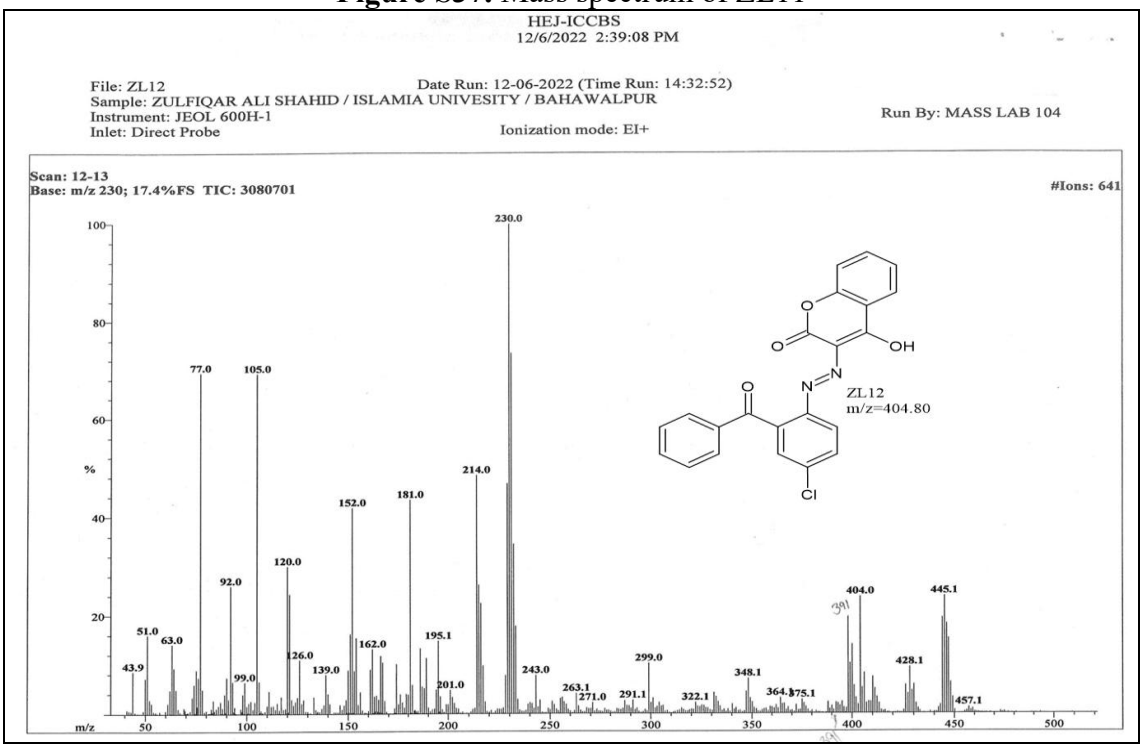

Figure S38. Mass spectrum of ZL12

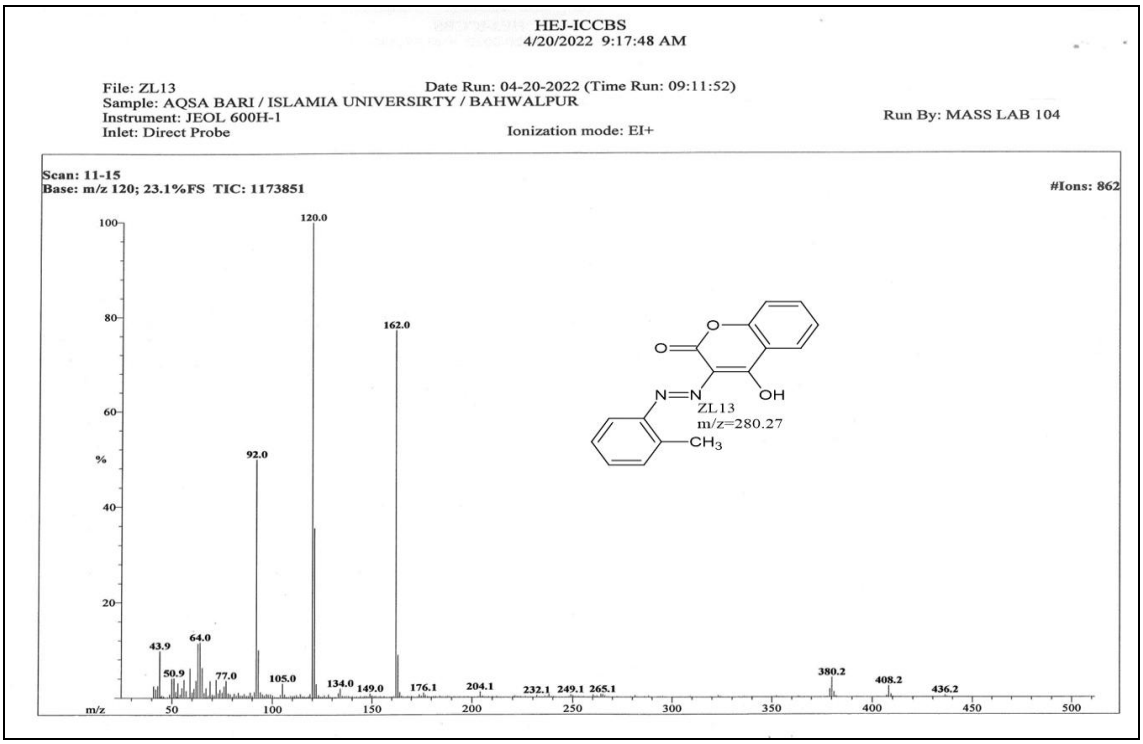

Figure S39. Mass spectrum of ZL13

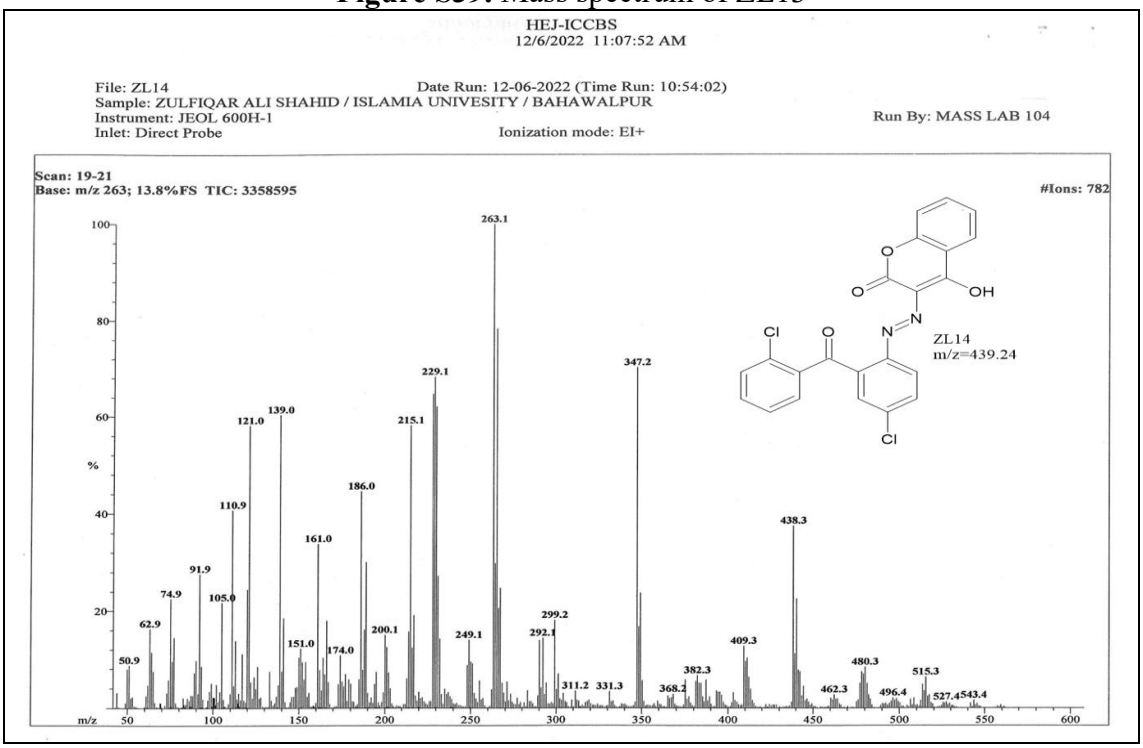

Figure.S40. Mass spectrum of ZL14

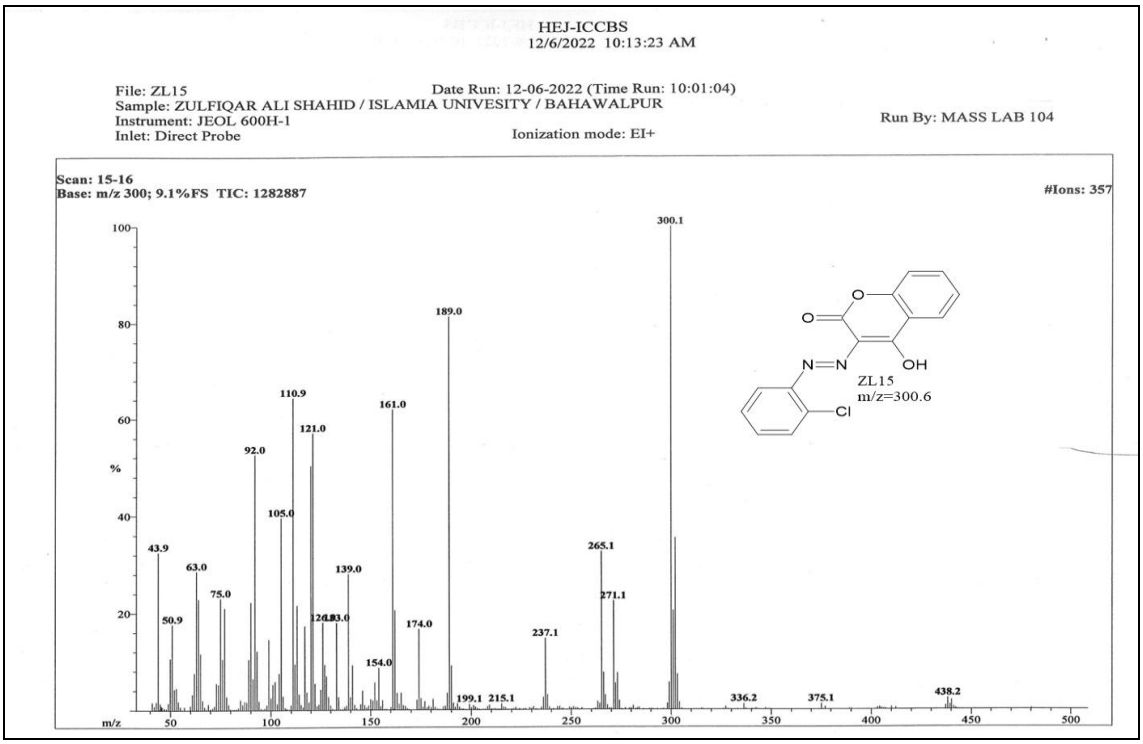

Figure.S41. Mass spectrum of ZL15

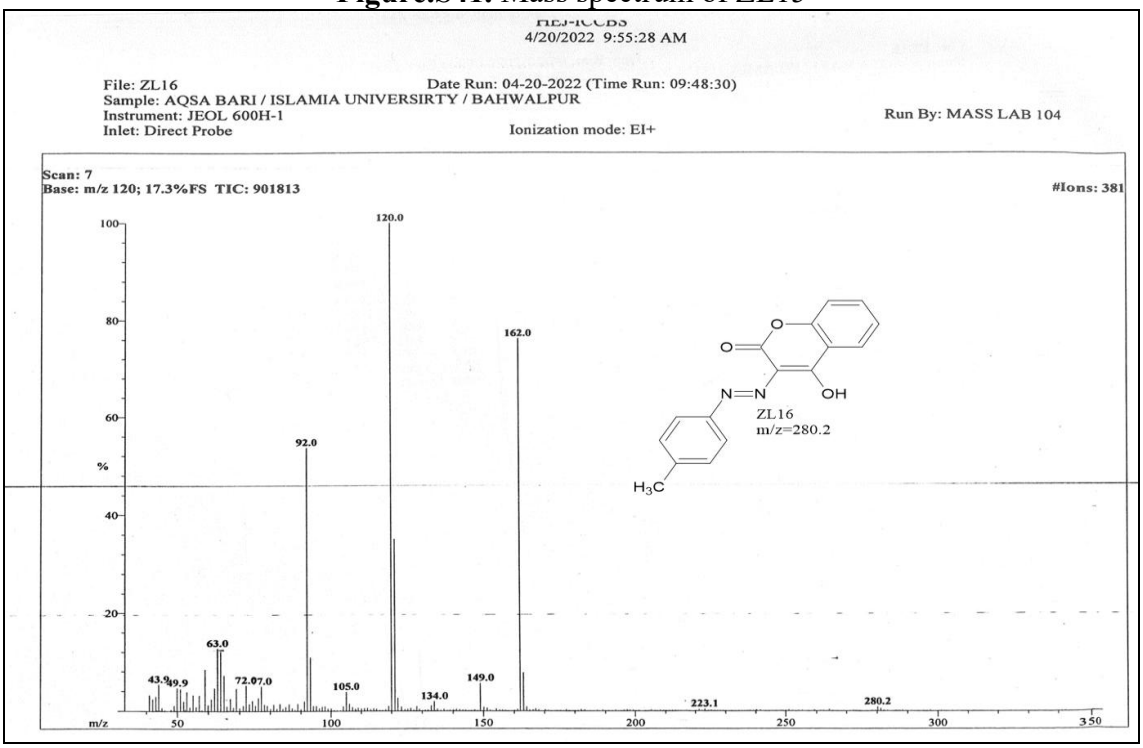

Figure.S42. Mass spectrum of ZL16