

# Supporting Information

## Preparation, Spectroscopic Characterization, Theoretical Investigations and *In Vitro* Anticancer Activity of Cd(II), Ni(II), Zn(II) and Cu(II) Complexes of 4(3*H*)-Quinazolinone Derived Schiff Base

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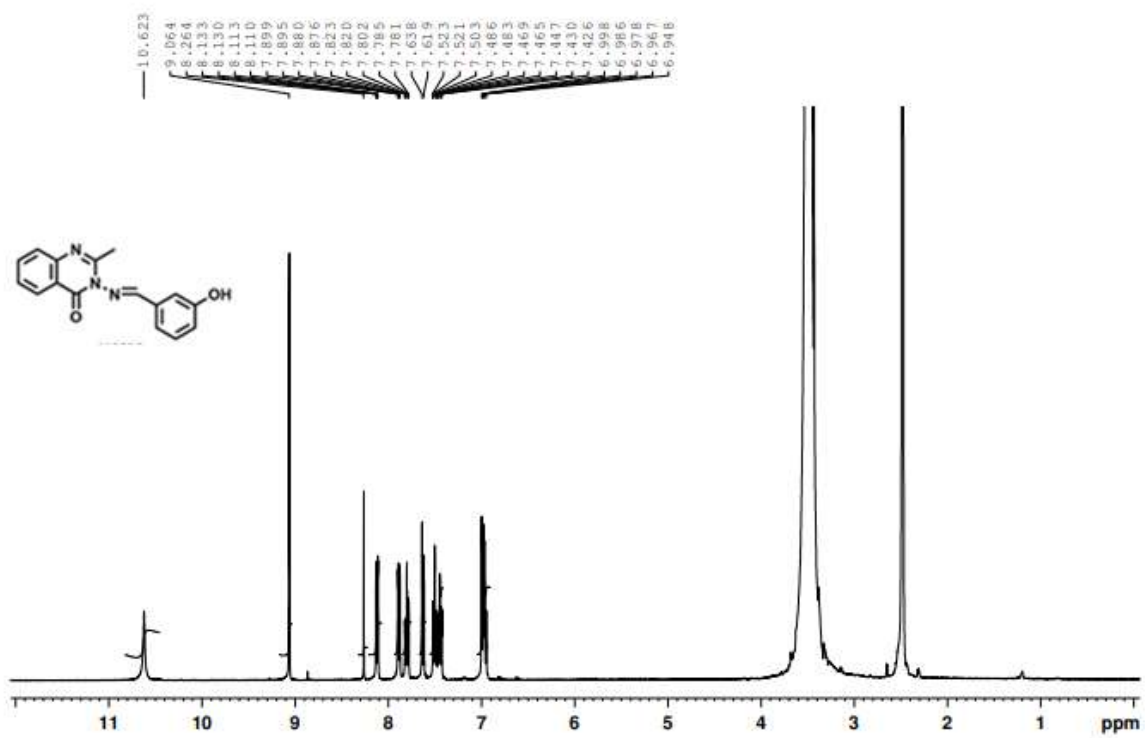


Figure S1: <sup>1</sup>H-NMR spectrum of HMAQ ligand.

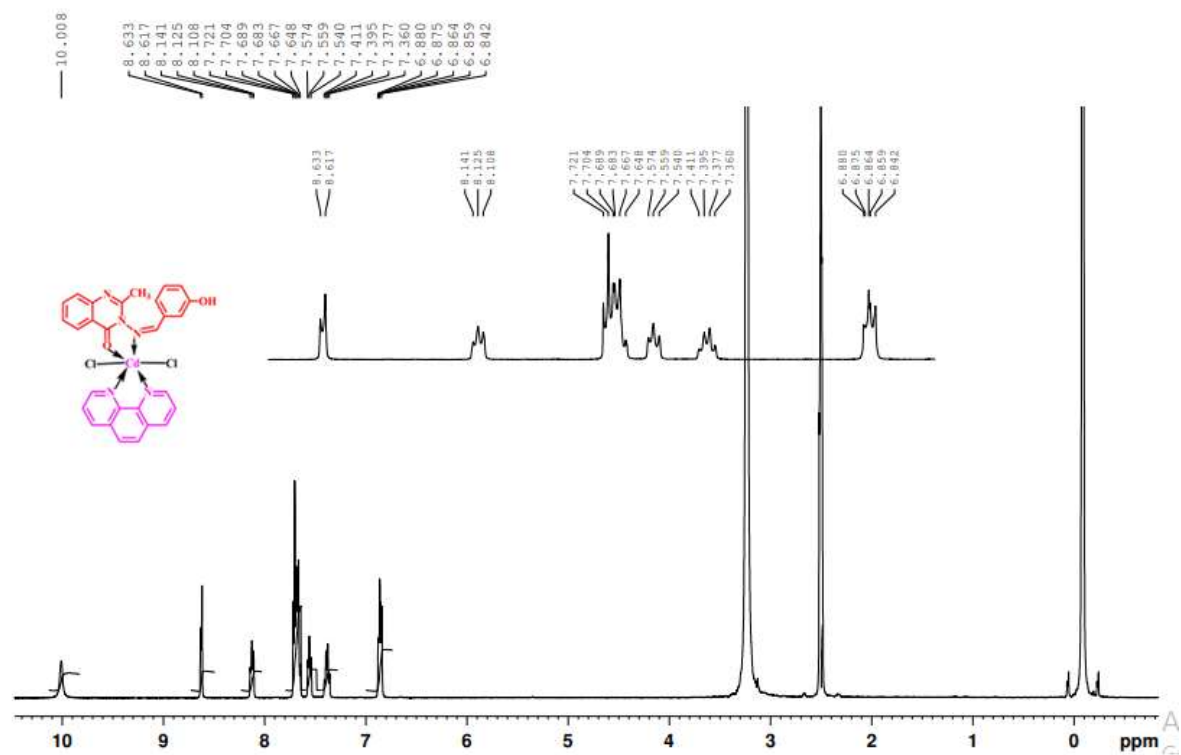


Figure S2:  $^1H$ -NMR spectrum of  $C_1$ .

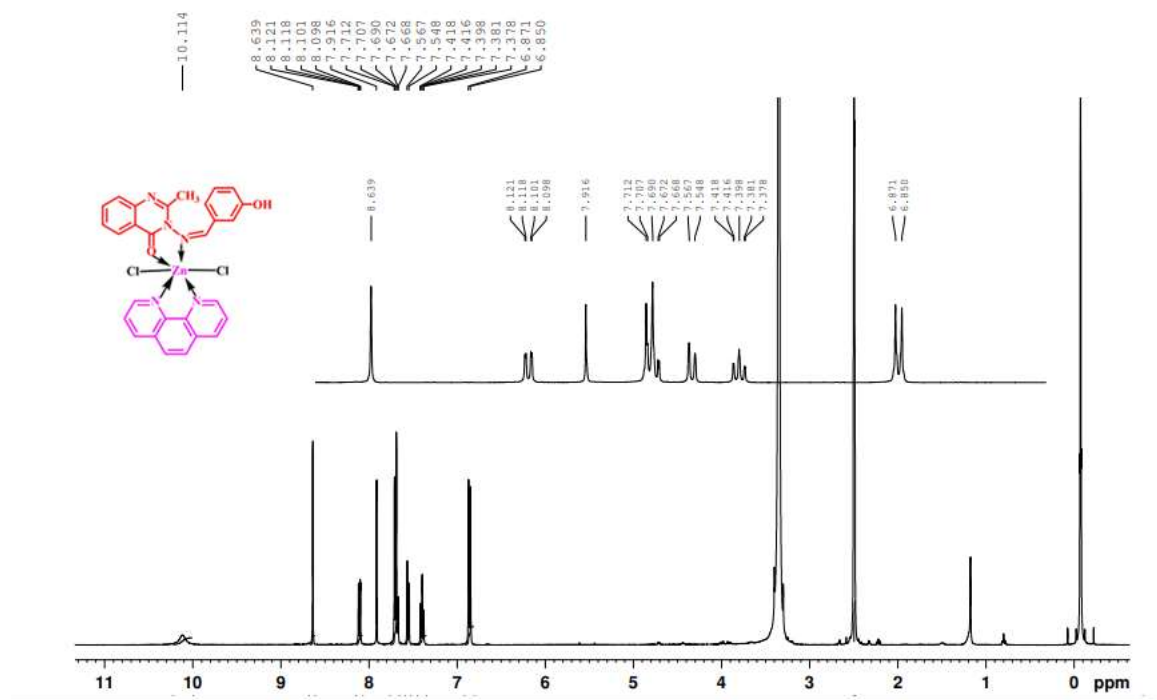


Figure S3: <sup>1</sup>H-NMR spectrum of C<sub>3</sub>.

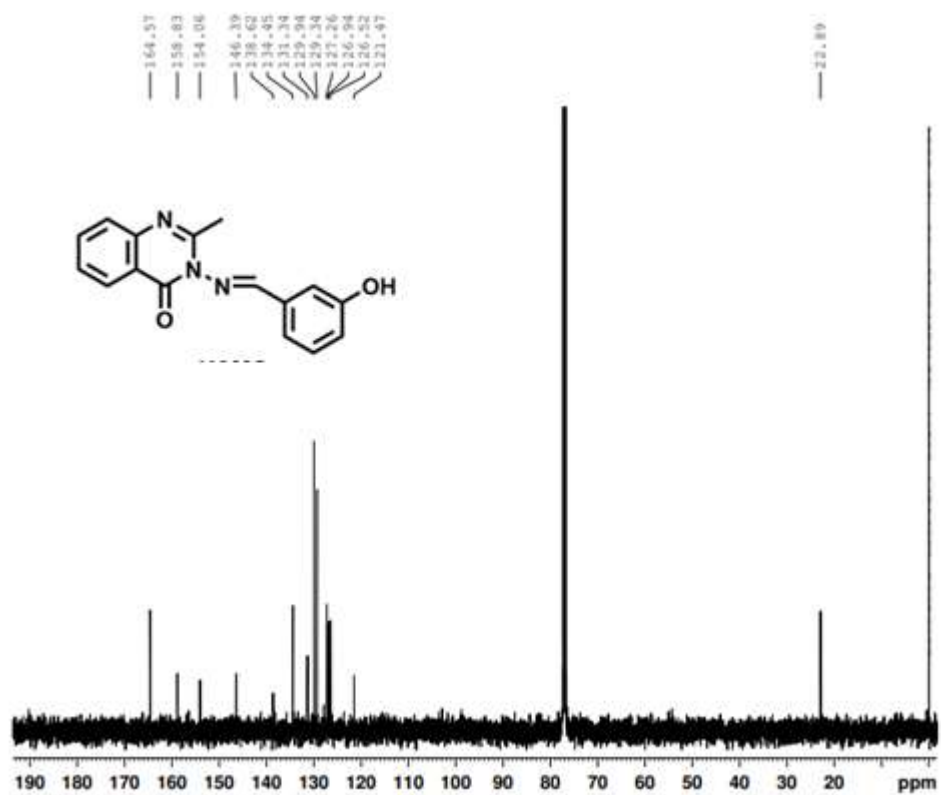


Figure S4: <sup>13</sup>C-NMR spectrum of HAMQ.

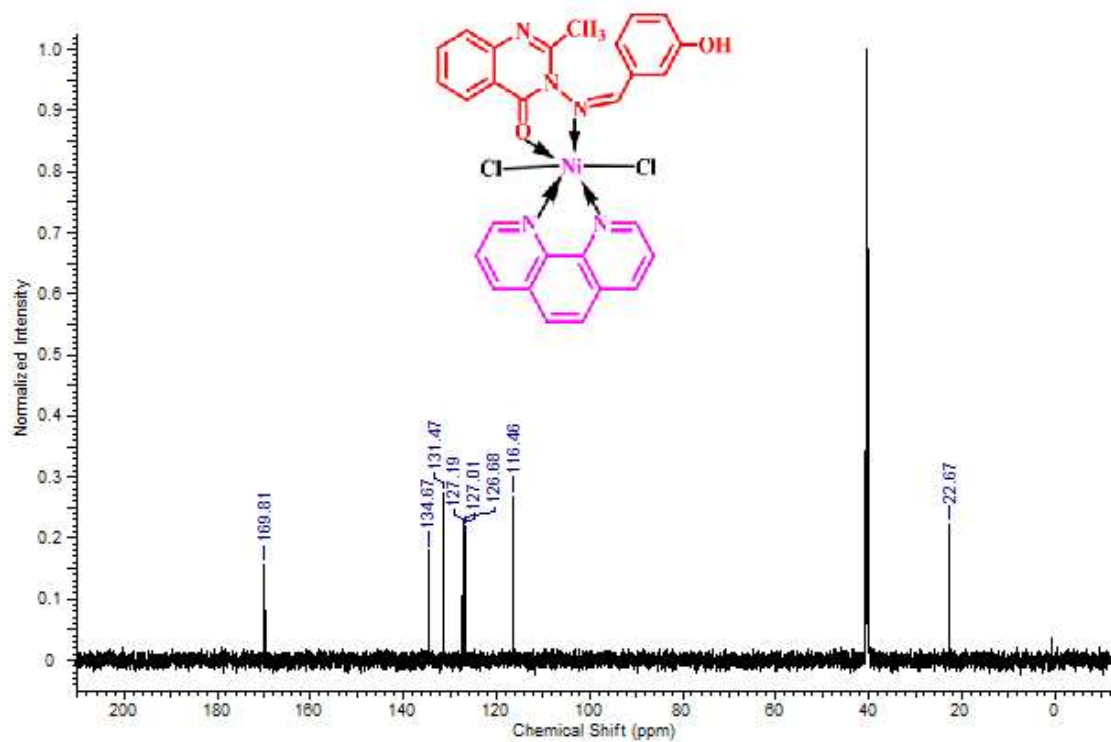
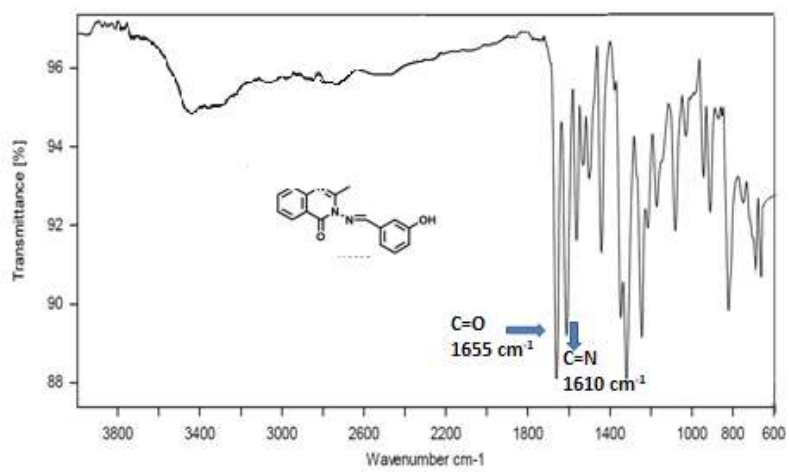
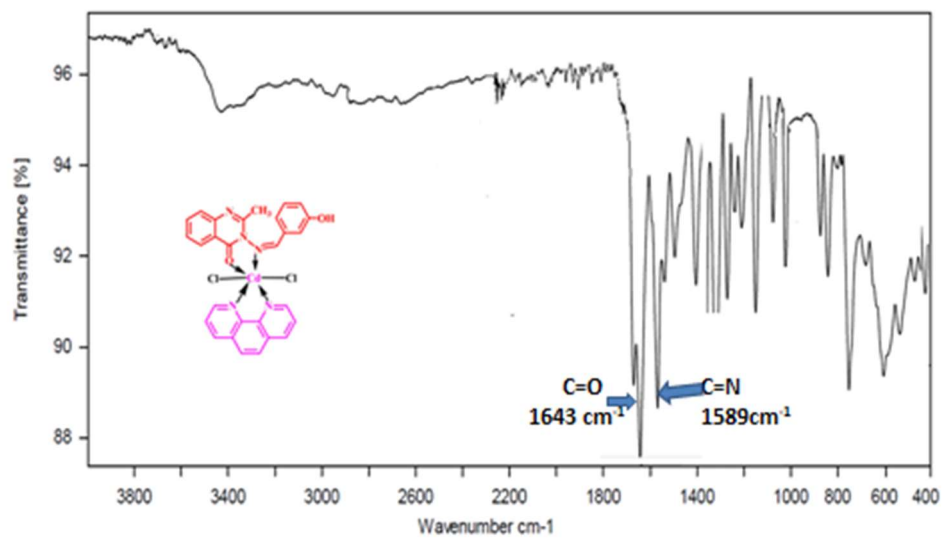


Figure S4:  $^{13}\text{C}$ -NMR spectrum of  $\text{C}_2$ .

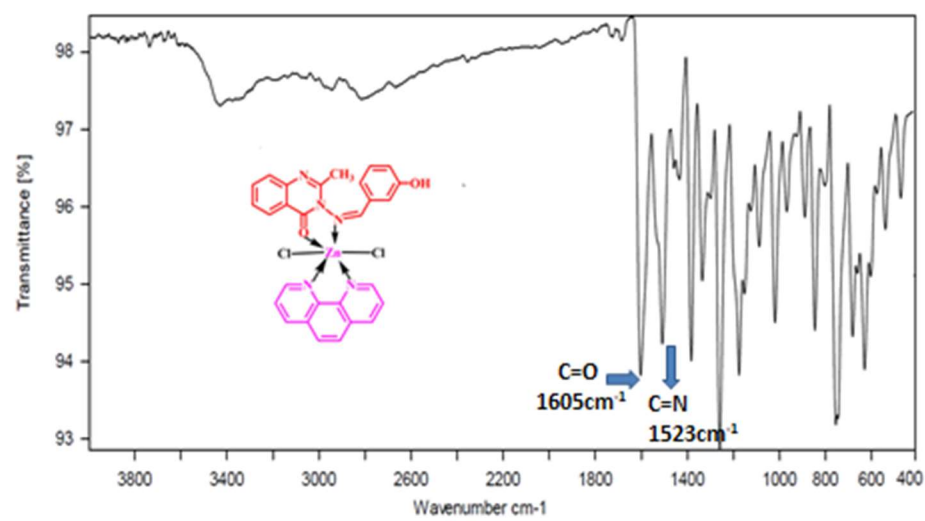


**Figure S6:** FT-IR spectrum of **HAMQ** ligand.

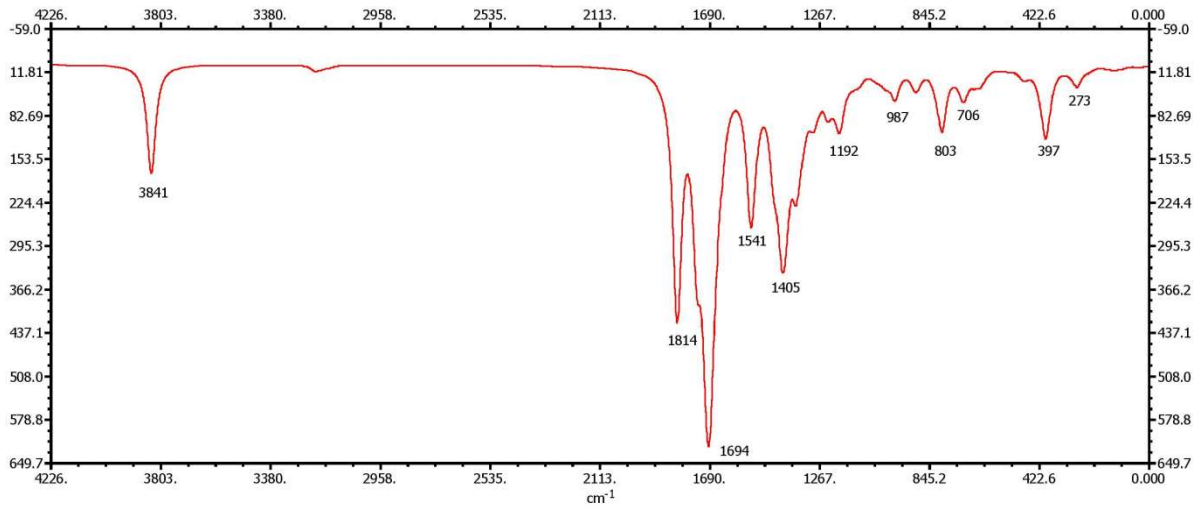




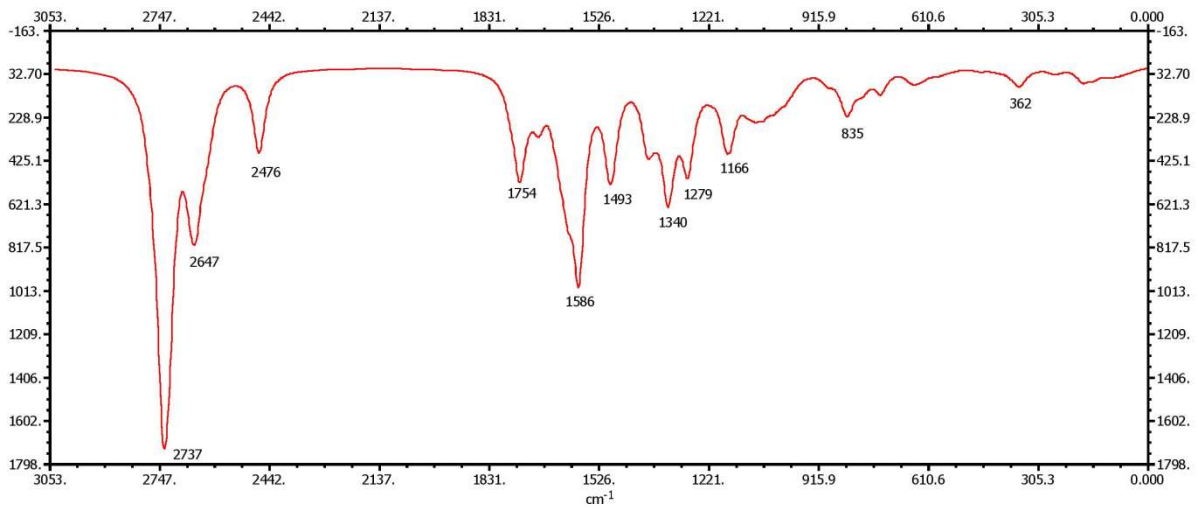
**Figure S7:** FT-IR spectrum of C<sub>1</sub>.



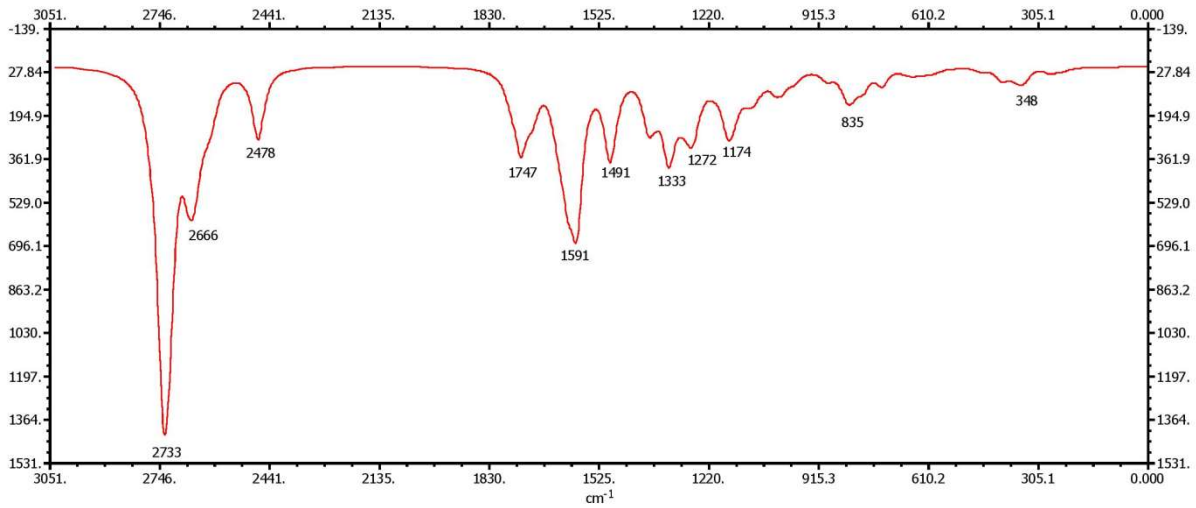
**Figure S8:** FT-IR spectrum of C<sub>3</sub>.



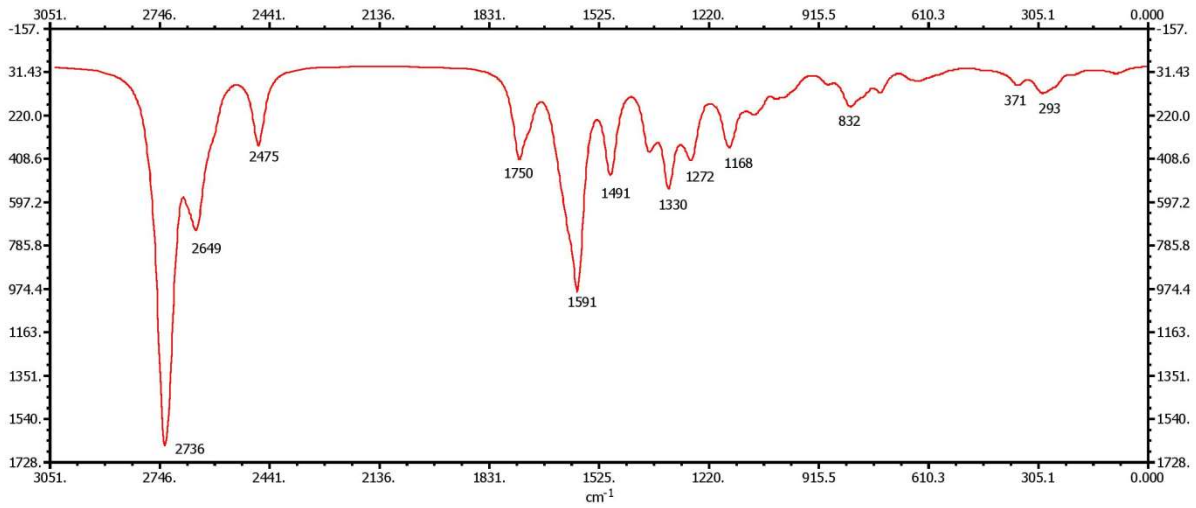
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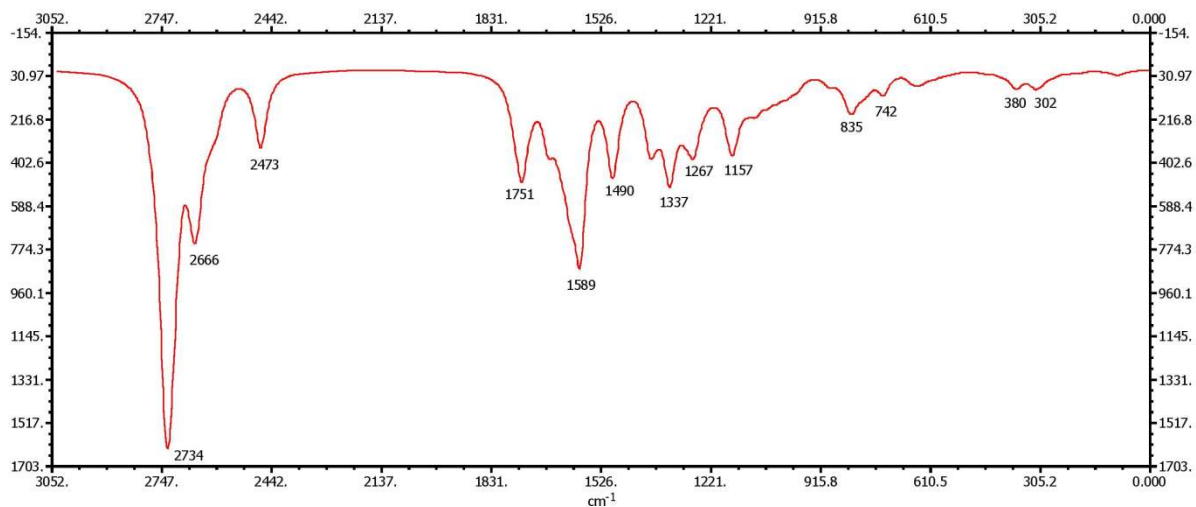
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(c)

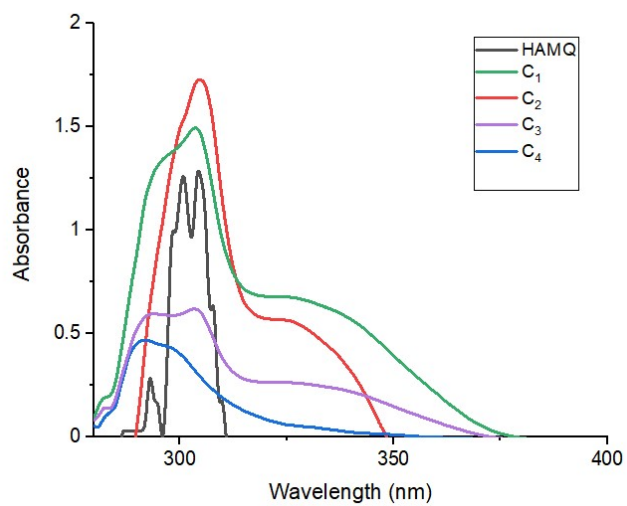


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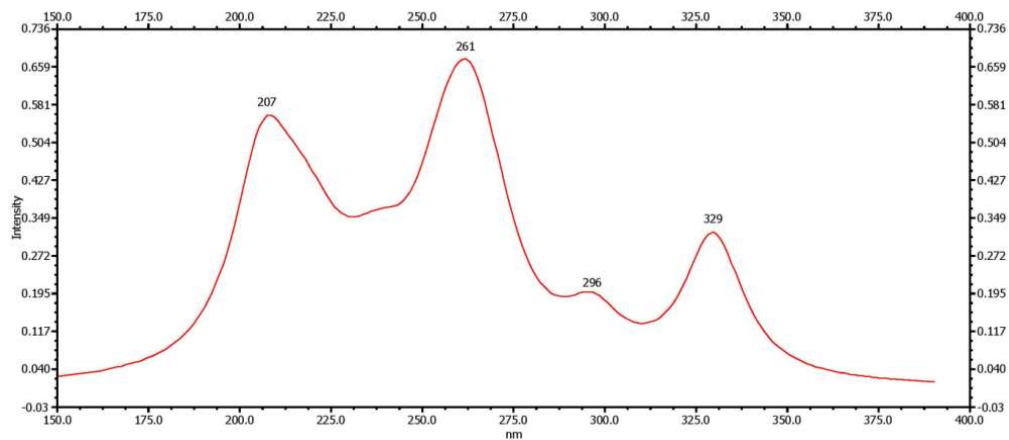


(e)

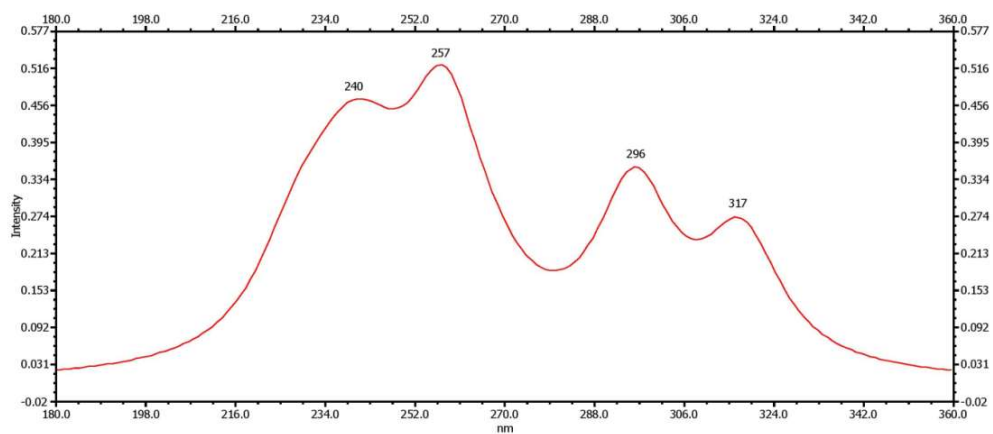
**Figure S9:** Graphical sketches of the simulated IR spectra of a) **HAMQ**, b)  $C_1$ , c)  $C_2$ , d)  $C_3$  and e)  $C_4$  complexes.



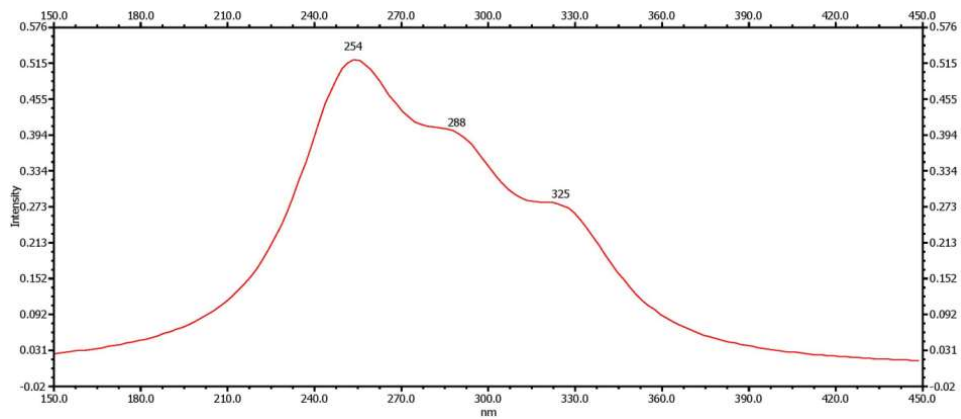
**Figure S10:** UV-Visible spectra of **HAMQ** and its complexes in DMSO solution.



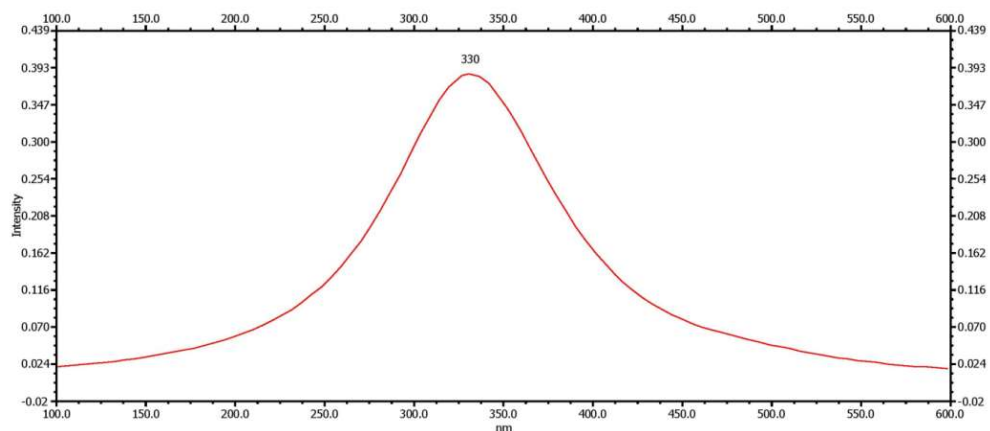
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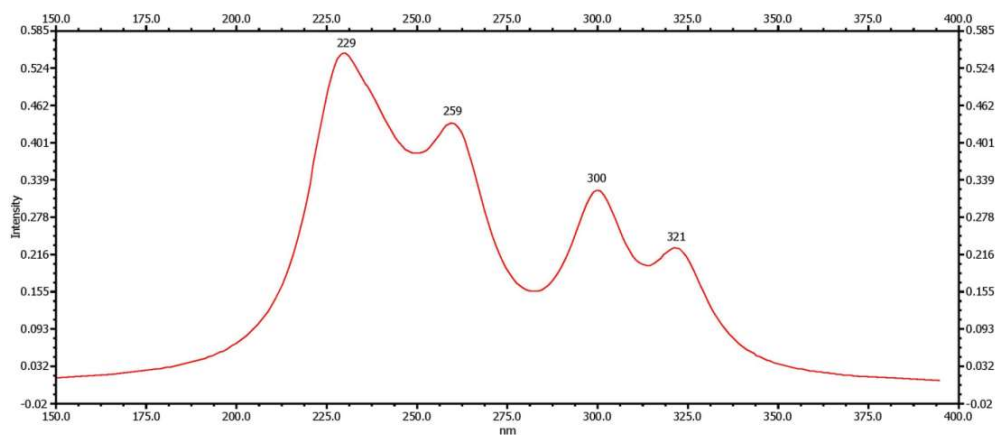
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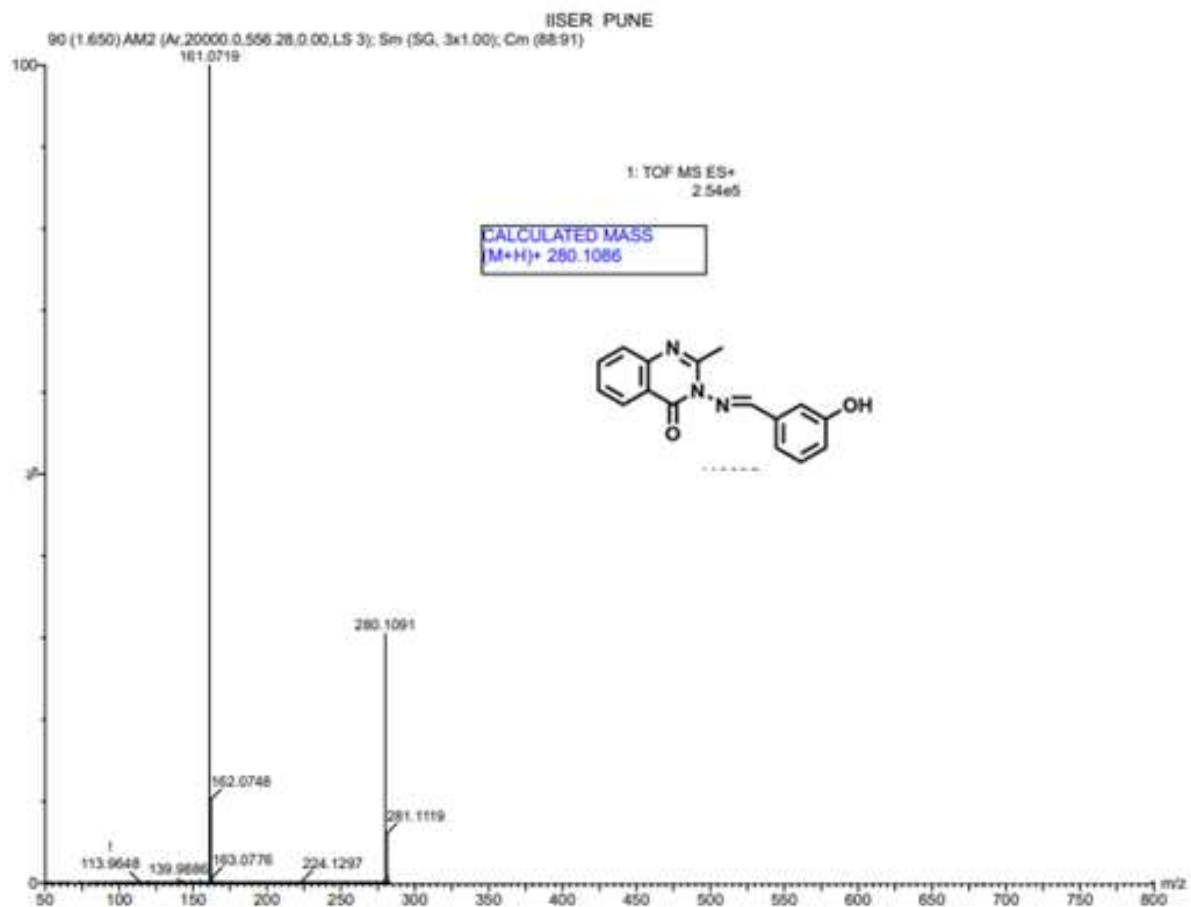
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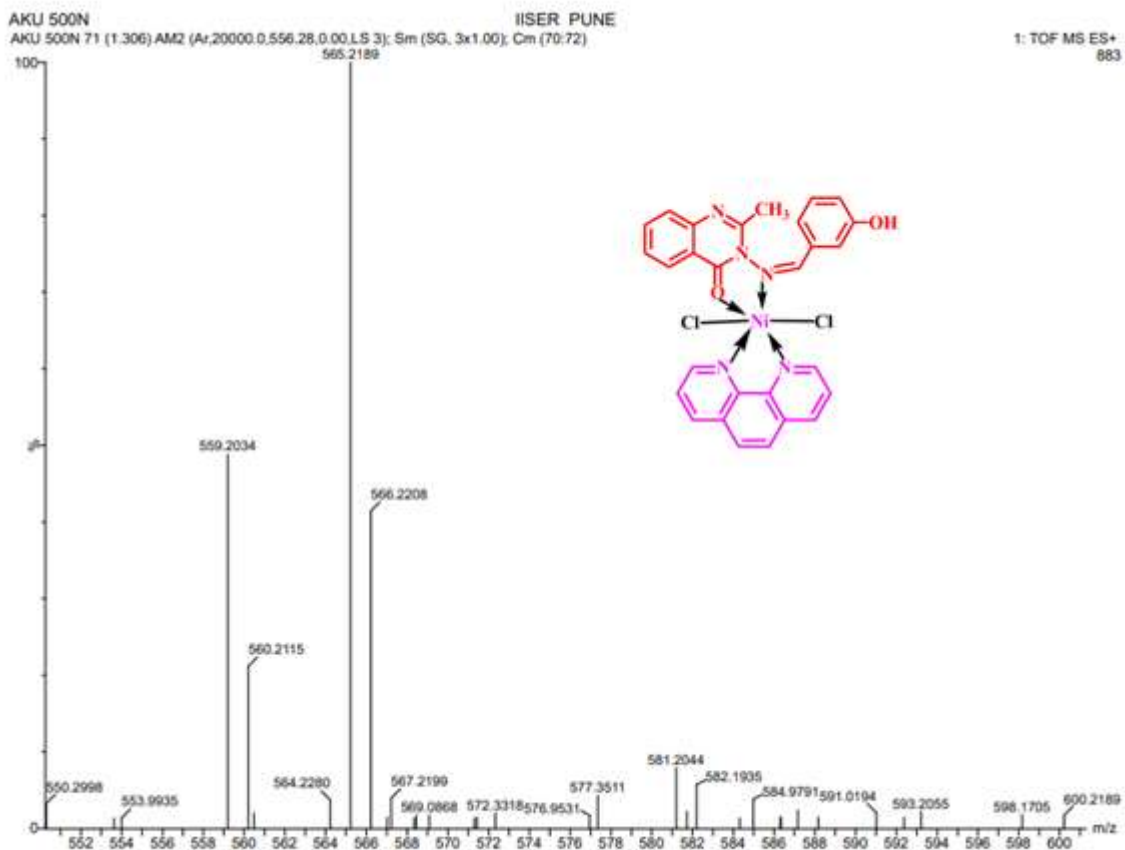
(e)

**Figure S11:** Graphical sketches of the UV-Visible spectra of a) **HAMQ**, b) **C1**, c) **C2**, d) **C3** and e) **C4** complexes.

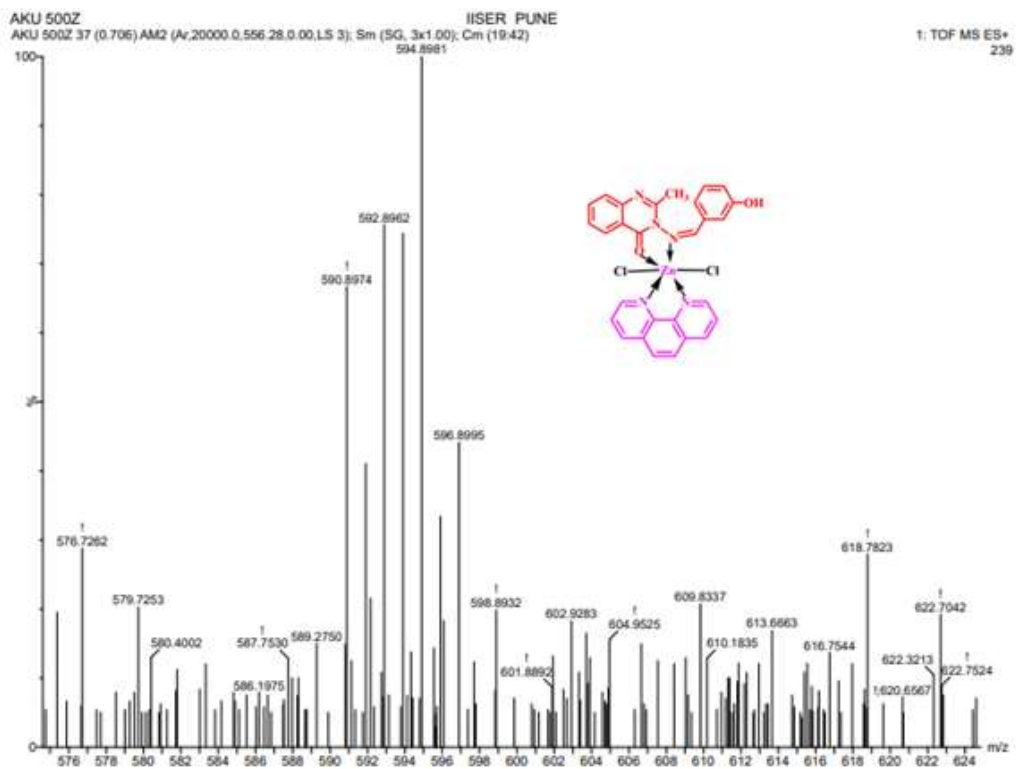




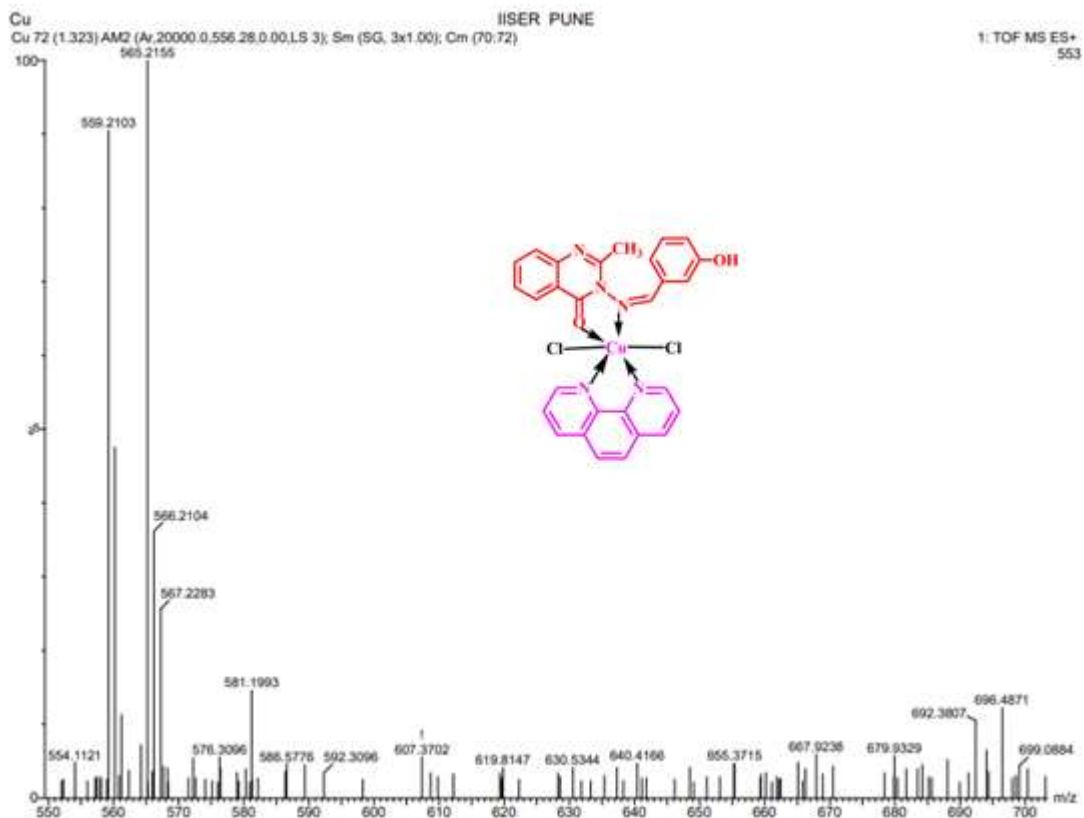
**Figure S12:** Mass spectrum of **HAMQ** ligand depicting [M+H]<sup>+</sup> at  $m/z = 281.1119$ .



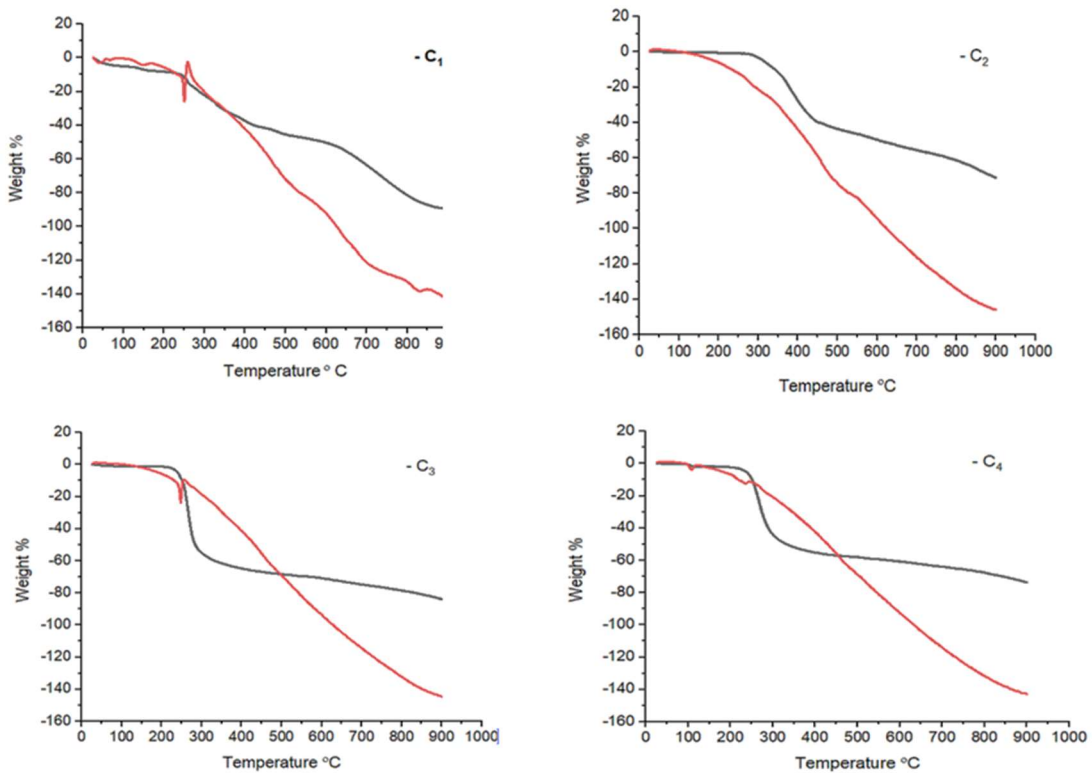
**Figure S13:** Mass spectrum of C<sub>2</sub> showing [M+2] at  $m/z = 591.0194$ .



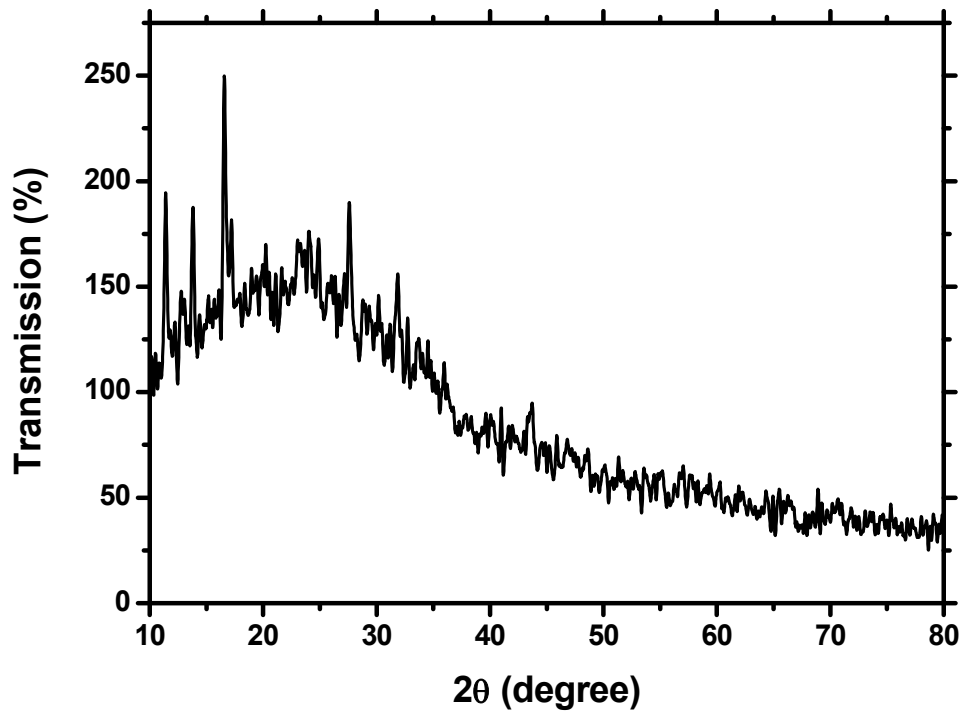
**Figure S14:** Mass spectrum of C<sub>3</sub> revealing [M]<sup>+</sup> at *m/z* = 594.8981.



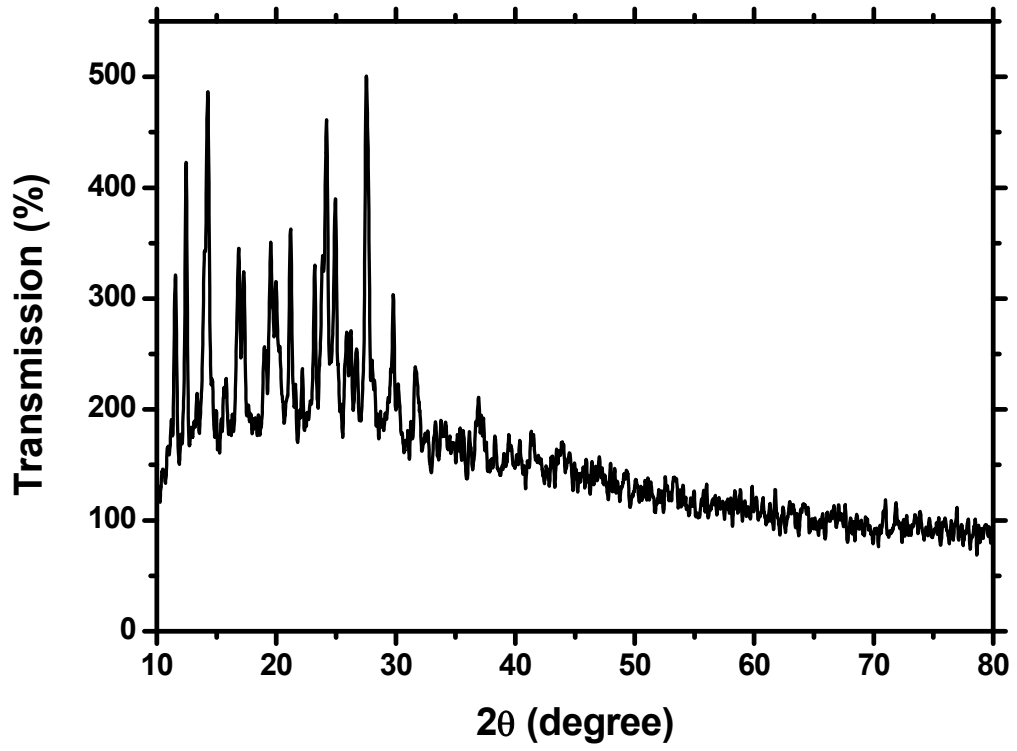
**Figure S15:** Mass spectrum of C<sub>4</sub> showing [M+2] at  $m/z = 592.3096$ .



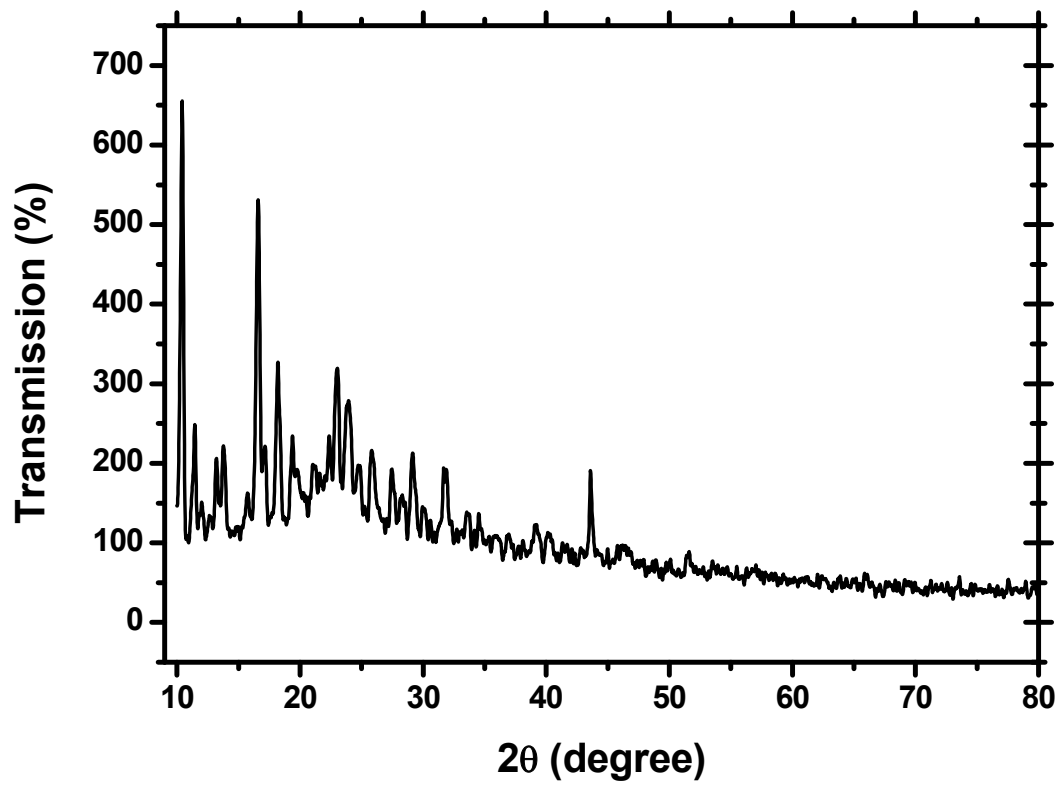
**Figure S16:** TGA/DTG curves of C<sub>1</sub>-C<sub>4</sub> complexes.



(a)

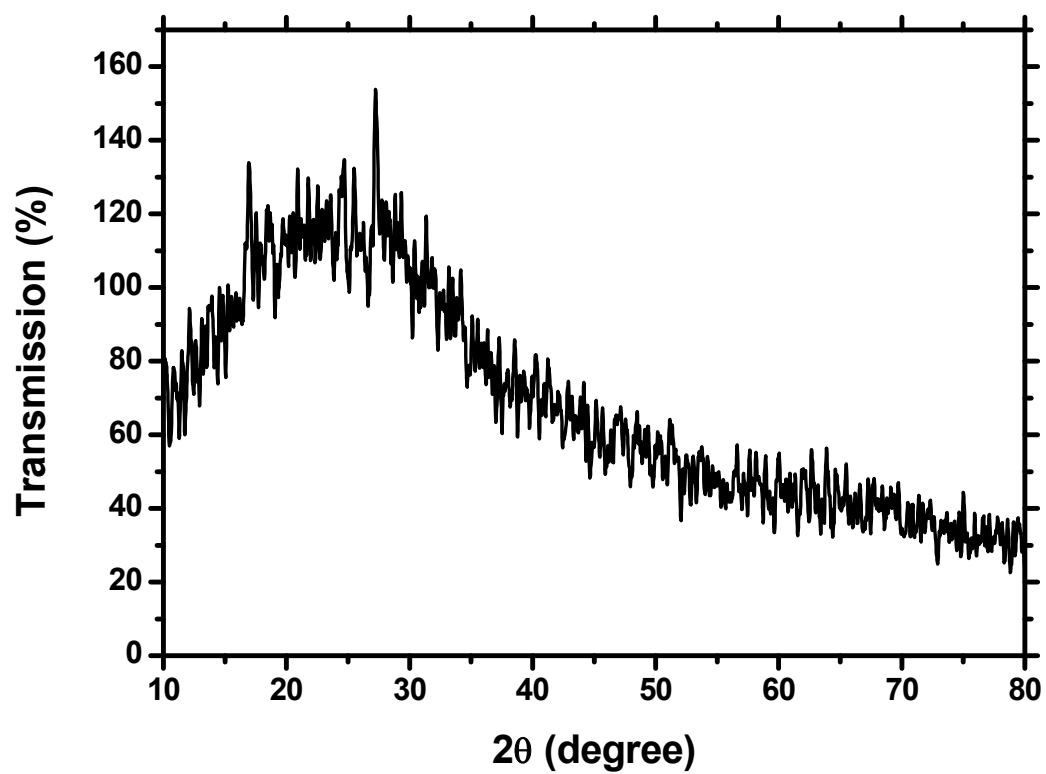


(b)



(c)





(d)

Figure S17: XRD pattern of C<sub>1</sub>-C<sub>4</sub> complexes.

**Table S1:** Analytical and physical data of the metal complexes.

Compound	Molecular Formula	Yield (%)	(Calculated) Found %				Molecular Conductance ( $\Omega^{-1} \text{cm}^2 \text{mol}^{-1}$ )
			C	H	N	M	
C1	$\text{C}_{28}\text{H}_{21}\text{N}_5\text{O}_2\text{Cl}_2$ Cd	63	(52.32) 52.19	(3.29) 3.66	(10.89) 10.74	(17.49) 17.60	24.08
C2	$\text{C}_{28}\text{H}_{21}\text{N}_5\text{O}_2\text{Cl}_2$ Ni	57	(57.84) 57.88	(3.84) 3.89	(12.82) 12.85	(9.84) 9.87	22.54
C3	$\text{C}_{28}\text{H}_{21}\text{N}_5\text{O}_2\text{Cl}_2$ Cu	64	(55.81) 55.93	(3.82) 3.91	(12.78) 12.97	(9.61) 9.72	17.93
C4	$\text{C}_{28}\text{H}_{21}\text{N}_5\text{O}_2\text{Cl}_2$ Zn	62	(56.44) 56.40	(3.56) 3.53	(11.75) 11.72	(10.98) 10.94	15.91

**Table S2:** Important IR spectral bands of HAMQ ligand and its metal complexes.

<b>Compound</b>	<b><math>\nu(-OH)</math></b>	<b><math>\nu(C=O)</math></b>	<b><math>\nu(HC=N)</math></b>	<b><math>\nu(M-O)</math></b>
HAMQ	3005	1669	1601	-
C1	3226	1623	1588	540
C2	3219	1650	1588	536
C3	3221	1620	1592	538
C4	3300	1621	1588	533

**Table S3:** Important UV-vis spectral bands of HAMQ ligand and its metal complexes.

Compound	$\lambda_{\text{max}}$ in nm	$\epsilon_{\text{max}}$ in $\text{M}^{-1} \text{cm}^{-1}$
HAMQ	298, 301, 307	33557, 33222, 32573
C2	690	14493
C3	678,709	14749, 14085
C4	712	14045

**Table S4:** Stepwise thermal degradation of metal complexes.

Compound	Thermogravimetry (TG)		Mass loss (%)		Decomposition product loss
	Stage	Temp (°C)	Found	Calculated	
C1	I	26-250	1.62	2.32	Cl Organic Moiety
	II	250-900	82.1	82.15	
C2	I	26-220	8.72	8.37	Cl 1,10-phen -N <sub>2</sub> Fraction of Ligand
	II	220-430	32.12	33.69	
		430-596	7.34	7.81	
		596-900	41.08	39.98	
C3	I	26-230	2.42	2.50	Cl Organic Moiety
	II	200-800	71.03	71.77	
C4	I	26-380	56.46	58.75	Fraction of Ligand Remaining moiety
	II	380-815	15.17	15.44	

**Table S5:** Crystallographic data of C<sub>1</sub>.

Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]	h	k	l
9.6171	19.54	0.2362	9.19658	48.91	0	1	1
11.406	21.24	0.2362	7.75792	100.00	0	1	2
13.8182	17.58	0.2362	6.40861	6.01	0	1	0
16.5771	30.86	0.1574	5.34774	5.74	0	0	2
19.775	24.1	0.1604	4.48955	13.23	1	2	1
21.6401	17.95	0.1564	4.10665	8.13	1	1	-1
23.0776	31.2	0.1536	3.85399	2.79	1	3	0
24.1017	21.8	0.9595	3.69251	1.57	1	3	3
27.6158	16.08	0.2362	3.2301	24.83	1	1	1
36.2206	10.3	0.2903	2.48006	3.13	1	0	-5
44.8974	14.2	0.0717	2.01888	1.44	2	6	5
51.32	3	0.09	1.78029	2.64	0	2	8
56.88	1	0.09	1.61877	3.19	1	-3	-4
59.3	1	0.09	1.55836	0.56	2	8	2



**Table S6:** Crystallographic data of C<sub>2</sub>.

Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]	<b>h</b>	<b>k</b>	<b>l</b>
11.5666	42.6	0.1574	7.65058	54.19	0	0	2
12.454	72.01	0.1181	7.10736	91.59	0	1	2
14.2804	64.09	0.2362	6.20219	81.51	0	1	0
16.8661	36.54	0.1968	5.25675	46.47	1	0	0
17.3023	36.62	0.1574	5.12518	46.58	1	0	1
19.5302	32.66	0.1968	4.54527	41.54	1	0	2
21.1981	40.74	0.1968	4.19127	51.82	1	-1	-2
23.2063	51.07	0.1181	3.83292	64.96	0	0	4
24.2202	65.65	0.1968	3.6747	83.5	0	1	5
24.9381	43.44	0.1968	3.57053	55.26	1	1	4
25.9935	12.43	0.3149	3.4279	15.81	0	2	1
26.7731	13.47	0.2362	3.32983	17.13	1	-1	-4
27.5036	78.62	0.1968	3.24303	100	1	0	4
29.7969	33.61	0.1574	2.99844	42.75	1	1	-2
31.7232	16.52	0.4723	2.82063	21.02	1	2	5

**Table S7:** Crystallographic data of C<sub>3</sub>.

Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]	<b>h</b>	<b>k</b>	<b>l</b>
10.4499	135.22	0.2755	8.46547	100	0	0	2
11.4571	40.09	0.1181	7.72342	29.65	0	1	2
13.1906	20.45	0.1968	6.71207	15.12	0	1	0
13.8191	25.61	0.2362	6.4082	18.94	0	1	3
16.6328	85.93	0.3149	5.32993	63.55	0	1	-1
18.1969	60.06	0.1968	4.87519	44.42	1	1	2
19.3392	19.87	0.3149	4.58973	14.69	1	1	1
21.1293	9.08	0.3936	4.20475	6.72	1	0	1
23.1285	29.75	0.2362	3.84563	22	1	2	2
24.051	22.61	0.4723	3.70018	16.72	0	2	1
25.8042	18.59	0.3936	3.45262	13.75	1	2	1
27.4571	15.08	0.3149	3.24841	11.15	1	2	7
29.1761	24.86	0.2362	3.06081	18.39	1	3	6
31.7671	16.4	0.3936	2.81684	12.13	0	0	6



**Table S8:** Crystallographic data of C<sub>4</sub>.

Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]	<b>h</b>	<b>k</b>	<b>l</b>
10.4499	135.22	0.2755	8.46547	100	0	0	2
11.4571	40.09	0.1181	7.72342	29.65	0	1	2
13.1906	20.45	0.1968	6.71207	15.12	0	1	0
13.8191	25.61	0.2362	6.4082	18.94	0	1	3
16.6328	85.93	0.3149	5.32993	63.55	0	1	-1
18.1969	60.06	0.1968	4.87519	44.42	1	1	2
19.3392	19.87	0.3149	4.58973	14.69	1	1	1
21.1293	9.08	0.3936	4.20475	6.72	1	0	1
23.1285	29.75	0.2362	3.84563	22	1	2	2
24.051	22.61	0.4723	3.70018	16.72	0	2	1
25.8042	18.59	0.3936	3.45262	13.75	1	2	1
27.4571	15.08	0.3149	3.24841	11.15	1	2	7
29.1761	24.86	0.2362	3.06081	18.39	1	3	6
31.7671	16.4	0.3936	2.81684	12.13	0	0	6

**Table S9:** IC<sub>50</sub> values of all the synthesized compounds.

W/V*	C1	C2	C3	C4	HAMQ
	IC <sub>50</sub> (μM)				
0.5	7.77	8.51	7.92	8.43	16.5
0.25	3.88	4.25	3.96	4.21	8.27
0.125	1.94	2.12	1.98	2.10	4.13
0.0625	0.97	1.06	0.99	1.05	2.06
0.03125	0.48	0.53	0.49	0.52	1.03
0.01562	0.24	0.26	0.24	0.26	0.51
0.00781	0.12	0.13	0.12	0.13	0.25
0.003905	0.06	0.06	0.06	0.06	0.12
0.001952	0.03	0.03	0.03	0.03	0.06
0.000976	0.01	0.01	0.01	0.01	0.03

\* W/V – weight by volume. The IC<sub>50</sub> is dependent on W/V

## Expressions used to calculate global reactivity descriptors

Electronegativity

$$\chi = -\frac{1}{2}(I + A) \approx \frac{1}{2}(\varepsilon_L + \varepsilon_H)$$

Global Hardness

$$\eta = (I - A) \approx (\varepsilon_L - \varepsilon_H)$$

Global Electrophilicity

$$\omega = \frac{\chi^2}{2\eta} = \frac{(I + A)^2}{4(I - A)} \approx \frac{(\varepsilon_L + \varepsilon_H)^2}{4(\varepsilon_L - \varepsilon_H)}$$

Electro donating Power

$$\omega^- = \frac{(3I + A)^2}{16(I - A)} \approx \frac{(3\varepsilon_H + \varepsilon_L)^2}{16\eta}$$

Electro accepting Power

$$\omega^+ = \frac{(I + 3A)^2}{16(I - A)} \approx \frac{(\varepsilon_H + 3\varepsilon_L)^2}{16\eta}$$

Net Electrophilicity

$$\Delta\omega^\pm = \omega^+ - (-\omega^-) = \omega^+ + \omega^-$$

where  $\varepsilon_H$  and  $\varepsilon_L$  are the energies of the HOMO and LUMO, respectively.