Supplementary information: Synthesis, Characterization, Antimicrobial and Antiproliferative Activity Evaluation of Cu(II), Co(II), Zn(II), Ni(II) and Pt(II) Complexes with Isoniazid-Derived Compound

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Table S1. Crystal data and summary of intensity data collectionand structure refinement for **HL**

Compound	HL
Empirical formula	$C_{14}H_{13}N_3O_3$
Formula weight	271.27
Temperature (K)	200
Crystal system	monoclinic
Space group	$P2_1/n$
a (Å)	7.5757(5)
b (Å)	16.2389(7)
c (Å)	10.8065(7)
α (°)	90
β (°)	109.973(6)
γ (°)	90
V(Å^3)	1249.46(13)
Z	4
$D_{calc.}$ (g/cm^3)	1.442
μ (mm^{-1})	0.104
F(000)	568.0
Crystal size (mm)	0.45 × 0.2 × 0.2
θmin, θmax (°)	4.73 to 50.052
Limiting indices	-9 ≤ h ≤ 8 -19 ≤ k ≤ 18 -12 ≤ l ≤ 12
Reflections collected / unique	6626 / 2197 [R(int) = 0.0242]
Data/restraints/parameters	2197/0/183
Goodness-of-fit on F^2	1.064
Final R_1, wR_2 [I>2sigma(I)]	0.0397, 0.0941
R_1, wR_2 (all data)	0.0514, 0.1020
Largest diff. peak/ hole (eÅ^{-3})	0.20/-0.22

Table S2. FAB mass spectral data of complexes **1 - 8**.

Molecular formula	Mw (g/mol)	Molecular ion peak $[M]^+$	The peaks due to complex fragmentation			
$[Cu(L)(Cl)]\cdot 2H_2O$ (**1**)	405	407.1	218.2	249.9	302.3	388.1
$[Cu(L)(CH_3COO)]$ (**2**)	392.5	394.9	219.0	302.3	333.1	356.5
$[Cu(L)(NO_3)]\cdot H_2O$ (**3**)	413.5	411.1	195.0	241.0	302.4	333.1
$[Cu(L)(ClO_4)]\cdot H_2O$ (**4**)	451	452.2	225.2	302.3	321.5	352.2
$[Co(L)_2]$ (**5**)	599	604.0	333.1	452.1	512.5	568.6
$[Zn(L)_2]$ (**6**)	605.4	605.1	195.1	218.2	374.0	567.2
[Ni(L)(Cl)] (**7**)	364.2	365.1	232.7	251.0	296.9	343.9
[Pt(L)(Cl)] (**8**)	500.5	501.2	241.0	294.1	330.5	452.1

Table S3. Cell viability of the MCF-7, SKBR-3, A375 and NCI-H1573 cancer cells after 48 hours treatment with **HL** and the complexes.

		HL	1	2	3	4	5	6	7	8	DMSO	Py	Control
MCF-7	Viability %	21.53	2.47	2.10	2.44	3.43	55.61	17.72	47.75	21.71	77.79	74.39	100.00
	STD	1.83	0.70	0.65	1.06	1.57	6.57	1.01	5.19	2.37	2.89	8.87	0.20
SKBR-3	Viability %	76.26	25.24	6.88	62.65	48.72	76.68	61.43	21.11	85.27	78.90	77.51	100.00
	STD	1.40	15.30	1.99	5.01	3.88	10.59	0.85	6.53	1.66	3.58	2.12	0.20
A375	Viability %	82.43	84.43	0.73	1.59	0.70	88.96	71.66	98.97	73.45	101.48	81.57	100.00
	STD	1.90	2.57	0.27	0.53	1.02	3.60	2.15	2.14	1.03	6.67	10.71	0.40
NCI-H1573	Viability %	29.16		7.22	12.14	10.05	89.79	33.77		20.34	91.88	81.84	100.00
	STD	5.26		0.39	0.99	3.45	8.11	5.10		2.08	2.85	5.78	0.30

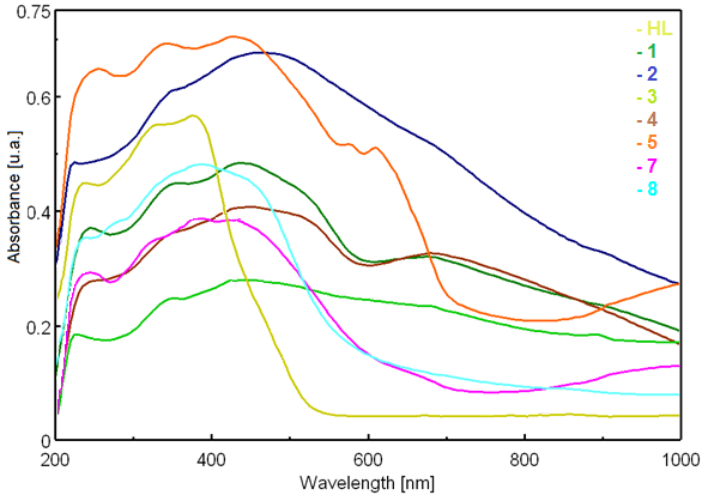


Figure S1. Electronic spectra of the ligands **HL** and metal complexes **1 – 5**, **7**, **8.**

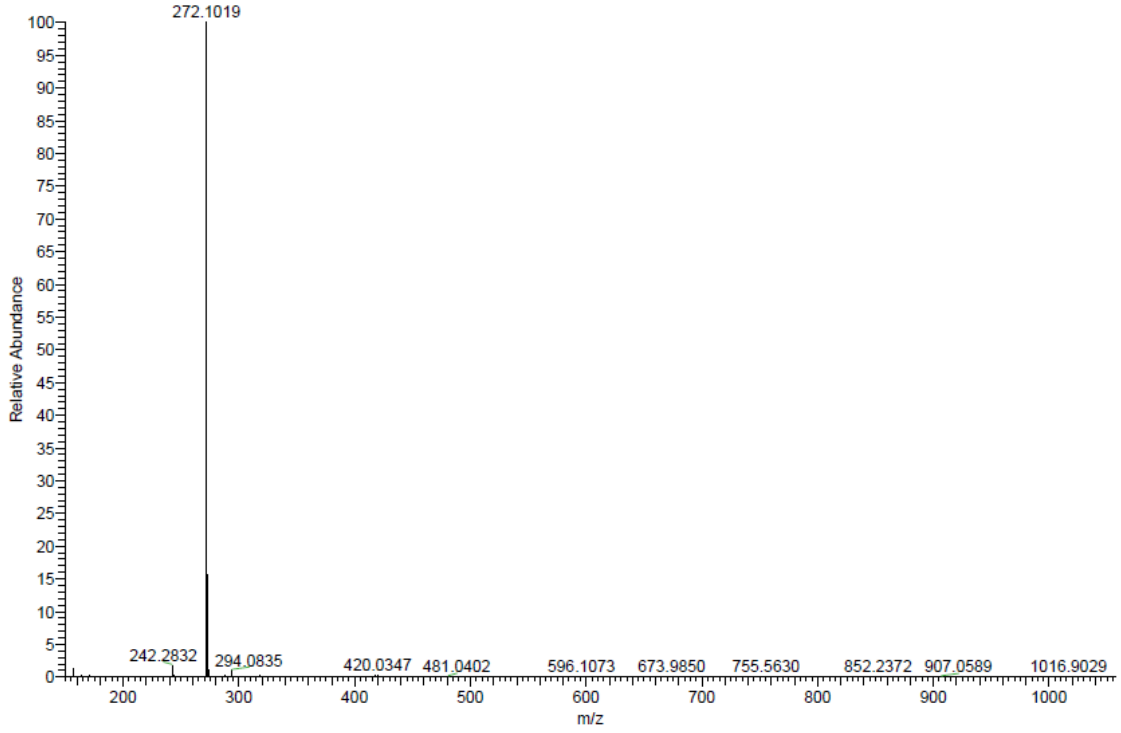
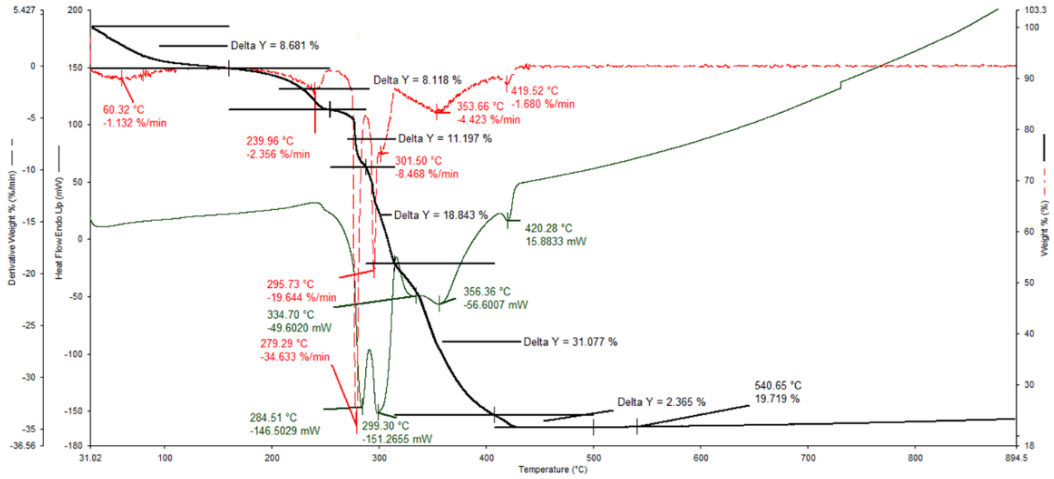
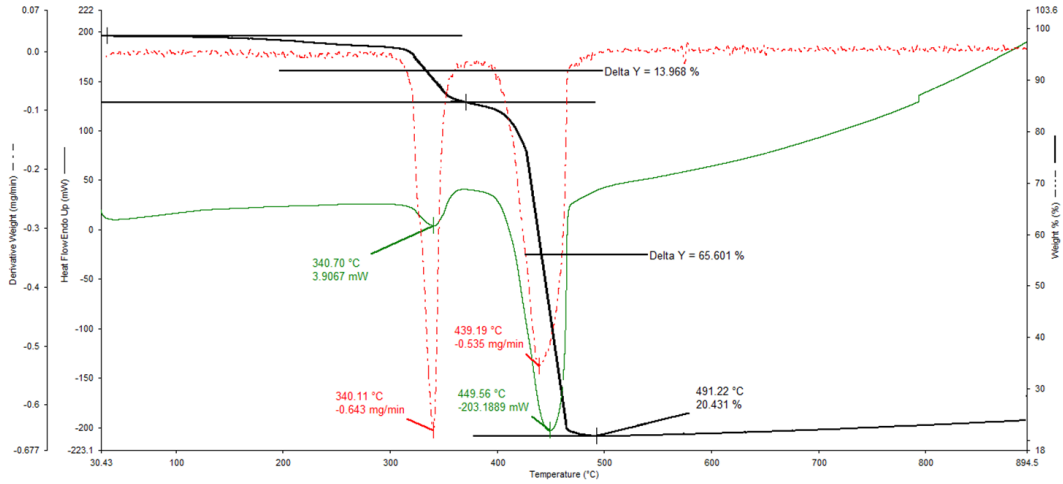


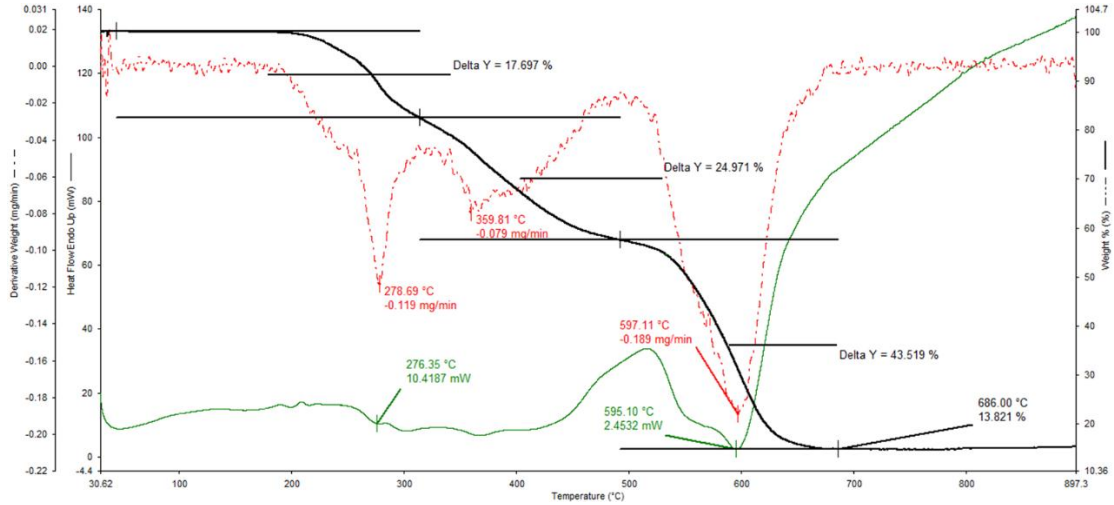
Figure S2. Mass spectrum of ligand **HL**



(a)



(b)



(c)

Figure S3. Thermogravimetric analysis of complexes (a)**1**, (b)**2** and (c)**6**.

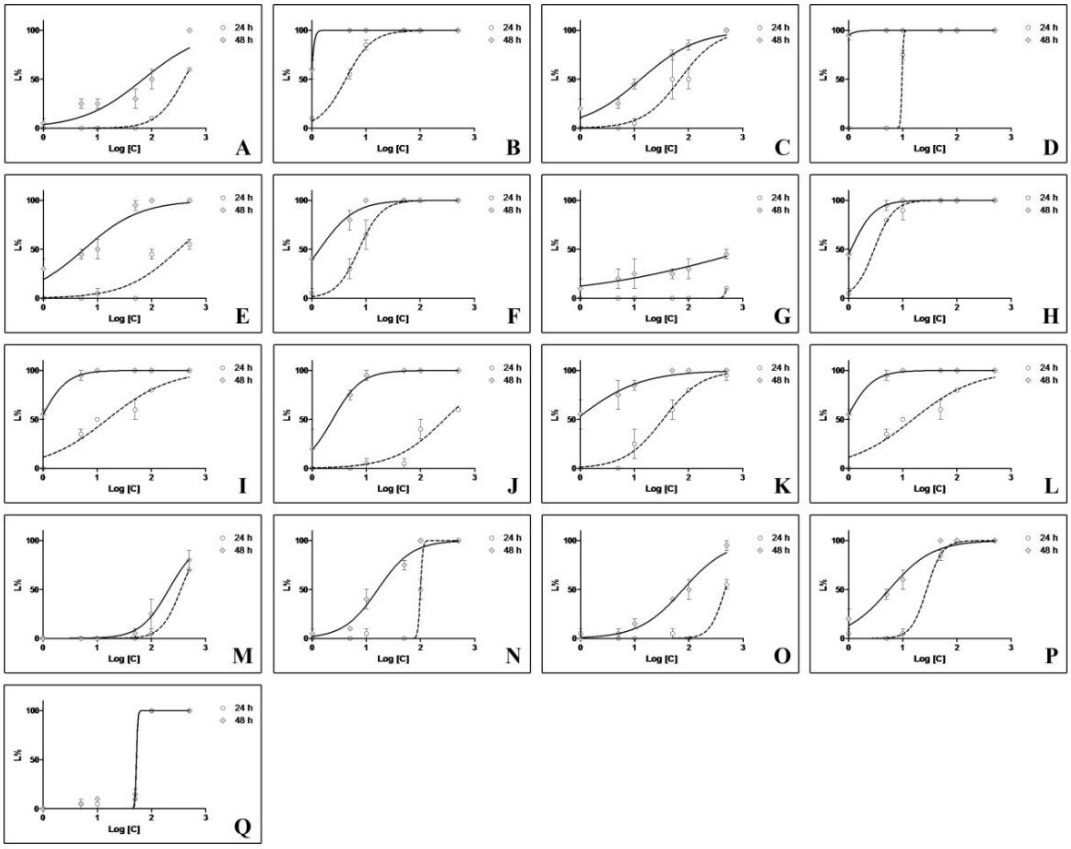


Figure S4. Concentration-lethality curves for toxicity assessment on *Daphnia magna* of (A) **1**, (B) $CuCl_2$, (C) **2**, (D) $Cu(CH_3COO)_2$, (E) **3**, (F) $Cu(NO_3)_2$, (G) **4**, (H) $Cu(ClO_4)_2$, (I) **5**, (J) $CoCl_2$, (K) **6**, (L) $ZnCl_2$, (M) **7**, (N) $NiCl_2$, (O) **8**, (P) K_2PtCl_4 and (Q) **HL**.