Electronic Supplementary Material (ESI) for Dalton Transactions.

Crystal structure, DFT, spectroscopic and biological activity evaluation of analgin complexes with Co(II), Ni(II) and Cu(II)

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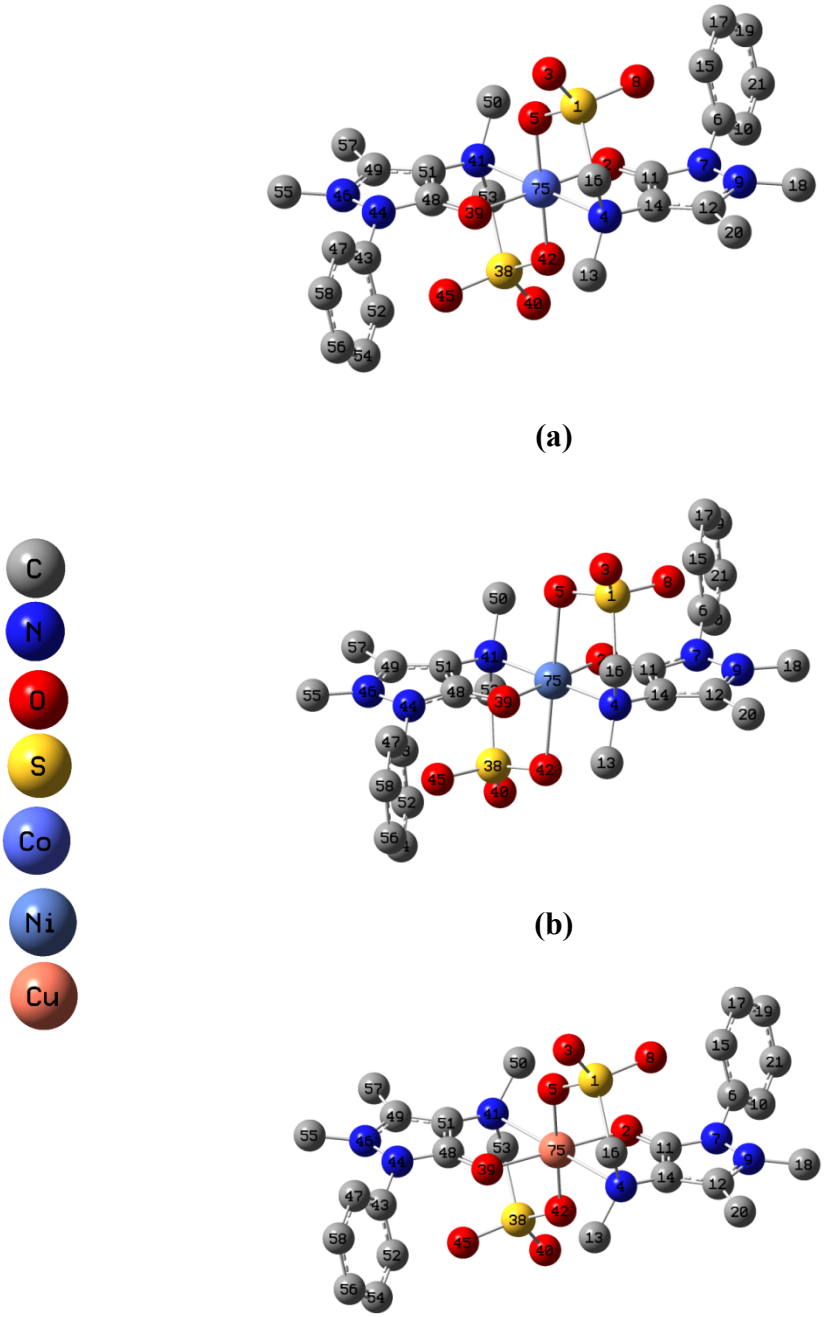
Supporting Information



(a)

(b)

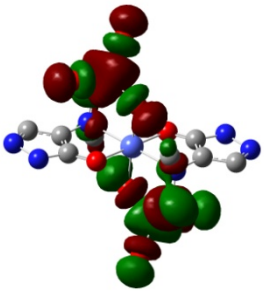
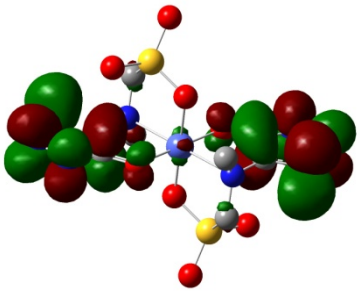
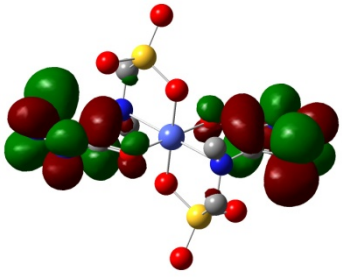
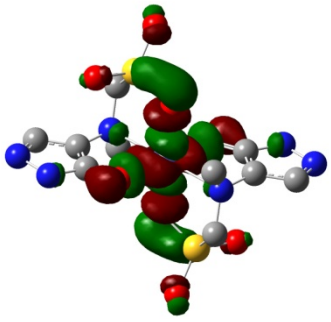
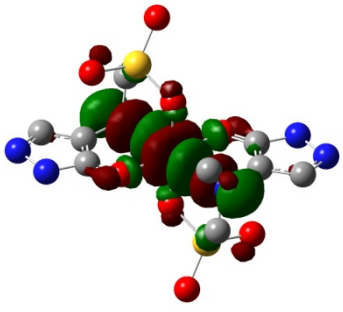
(c)

Fig. S1: Local minimum structures of complexes (a) **1**, (b) **2**, and (c) **3**, obtained at the DFT/B3LYP level of theory.

Table S1: Optimized bond length (Å) and angles (º) for complexes **1-3** at DFT/B3LYP level of theory					
1		**2**		**3**	
Bond length (Å)	Angles (º)	Bond length (Å)	Angles (º)	Bond length (Å)	Angles (º)
CoO2 = 1.983	O2CoN4 = 84.1	NiO2 = 1.922	O2NiN4 = 89.8	CuO2 = 2.002	O2CuN4 = 77.4
CoN4 = 2.388	O2CoO5 = 91.4	NiN4 = 2.051	O2NiO5 = 89.6	CuN4 = 2.724	O2CuO5 = 92.5
CoO5 = 1.942	O4CoO5 = 89.1	NiO5 = 2.467	O4NiO5 = 88.4	CuO5 = 1.952	O4CuO5 = 83.6
CoO39 = 1.983	O39CoN41 = 84.1	NiO39 = 1.922	O39NiN41 = 89.8	CuO39 = 2.002	O39CuN41 = 77.4
CoN41 = 2.388	O39CoO42 = 91.4	NiN41 = 2.051	O39NiO42 = 89.6	CuN41 = 2.724	O39CuO42 = 92.5
CoO42 = 1.942	N41CoO42 = 89.1	NiO42 = 2.467	N41NiO42 = 88.4	CuO42 = 1.952	N41CuO42 = 83.6

Table S2: Computed excitation energies (eV), electronic transition configurations and oscillator strengths (*f*) of the studied complexes (selected, (*f* > 0.001)			
λ (nm)	**E (eV)**	***f***	**Major contributions**
• **1**			
761	1.6272	0.0	H(β)→L+2(β) (13%)
533	2.3231	0.0	H(β)→L+3(β) (27%), H(β)→L+5(β) (35%)
484	2.5577	0.0	H-1(β)→L+2(β) (27%), H-1(β)→L+5(β) (23%)
335	3.7004	0.0055	H(β)→L(β) (86%)
307	4.0386	0.0007	H-1(α)→L+1(α) (46%)
• **2**			
484	2.5592	0.0002	H-1(α)→L(α) (48%), H-1(β)→L(β) (48%)
415	2.9812	0.0017	H-4(α)→L(α) (46%), H-4(β)→L(β) (46%)
409	3.0272	0.0011	H(α)→L+1(α) (49%), H(β)→L+1(β) (49%)
• **3**			
809	1.5314	0.0	H(β)→L(β) (38%)
569	2.1763	0.0064	H-1(β)→L(β) (97%)
526	2.3554	0.0067	H-3(β)→L(β) (89%)
462	2.6834	0.0131	H-4(β)→L(β) (65%)
426	2.9065	0.0164	H-7(β)→L(β) (68%)
347	3.5652	0.1172	H-13(β)→L(β) (81%)

Table S3: LUMO+3 to HOMO of [CoL_2] calculated by DFT/B3LYP method.

Orbital	Energy (eV)	Molecular orbital plot
LUMO+5	-0.60	
LUMO+3	-0.87	
LUMO+2	-0.99	
LUMO+1	-1.022	
LUMO	-1.044	

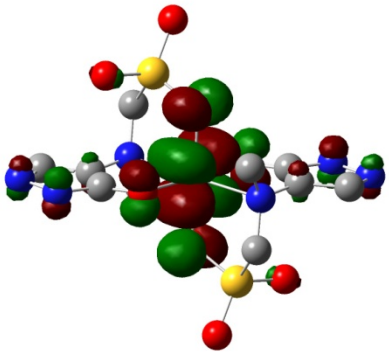
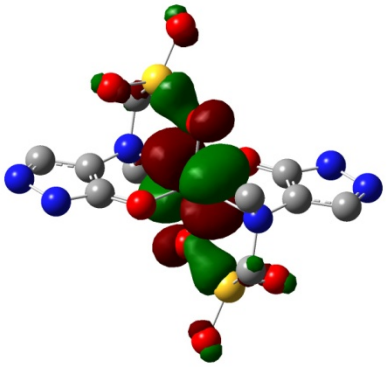
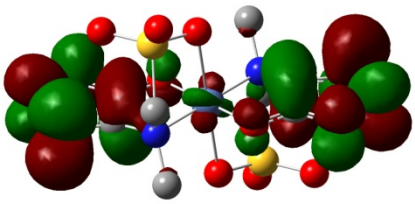
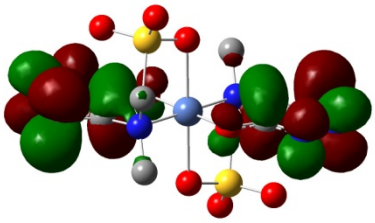
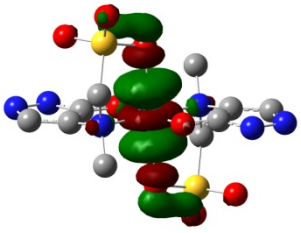
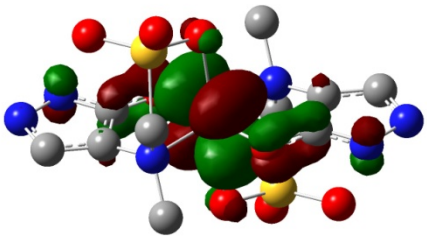
HOMO	-1.99	
HOMO-1	-5.83	

Table S4: LUMO+3 to HOMO of [NiL_2] calculated by DFT/B3LYP method.

Orbital	**Energy (eV)**	**Molecular orbital plot**
LUMO+1	-1.22	
LUMO	-2.34	
HOMO	-5.37	

HOMO-1	-6.06	
HOMO-4	-6.43