

Supporting data

Synthesis, DFT, biological and molecular docking analysis of novel manganese(II), iron(III), cobalt(II), nickel(II), and copper(II) chelate complexes ligated by 1-(4-nitrophenylazo)-2-naphthol

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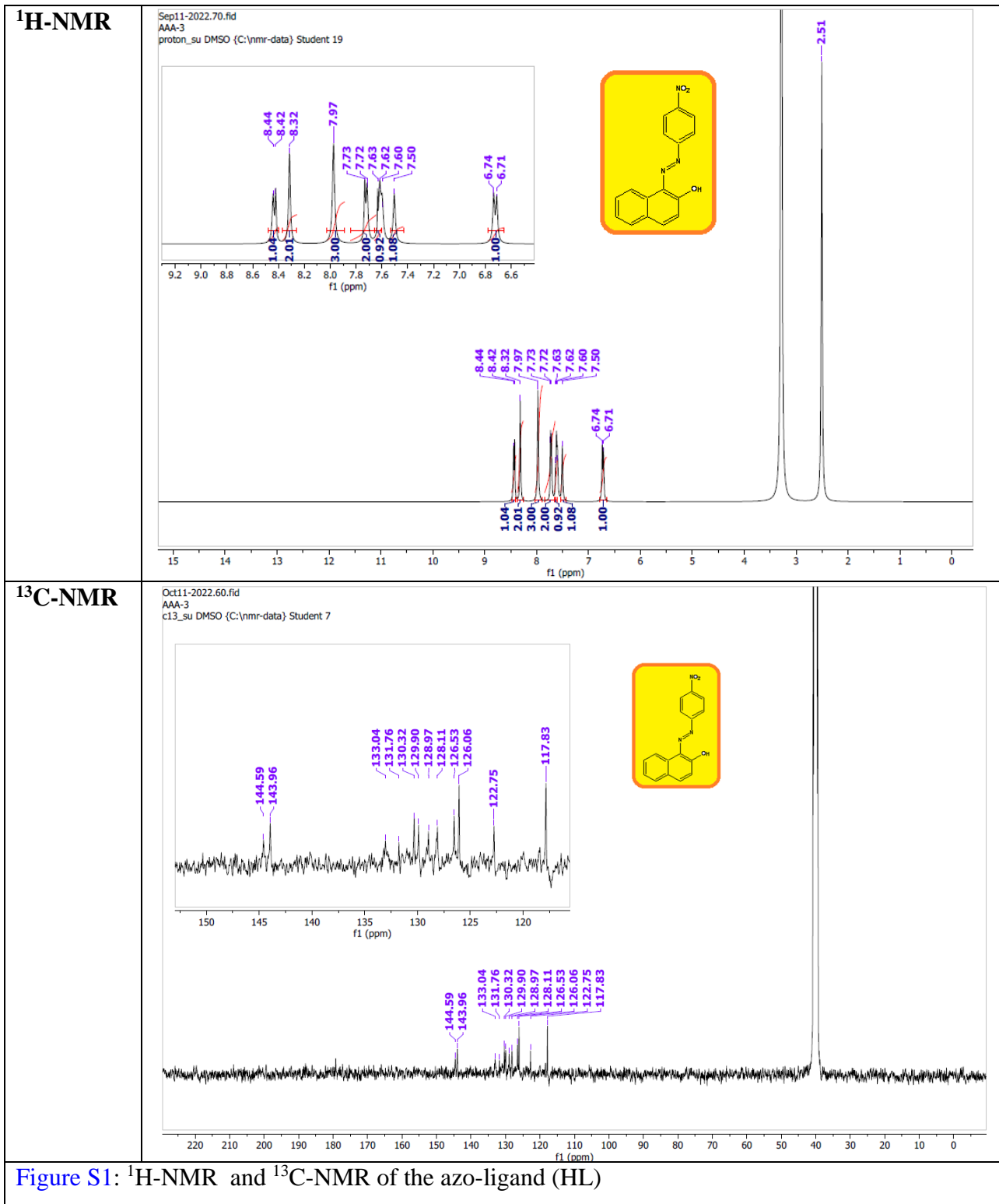
List of Figures;

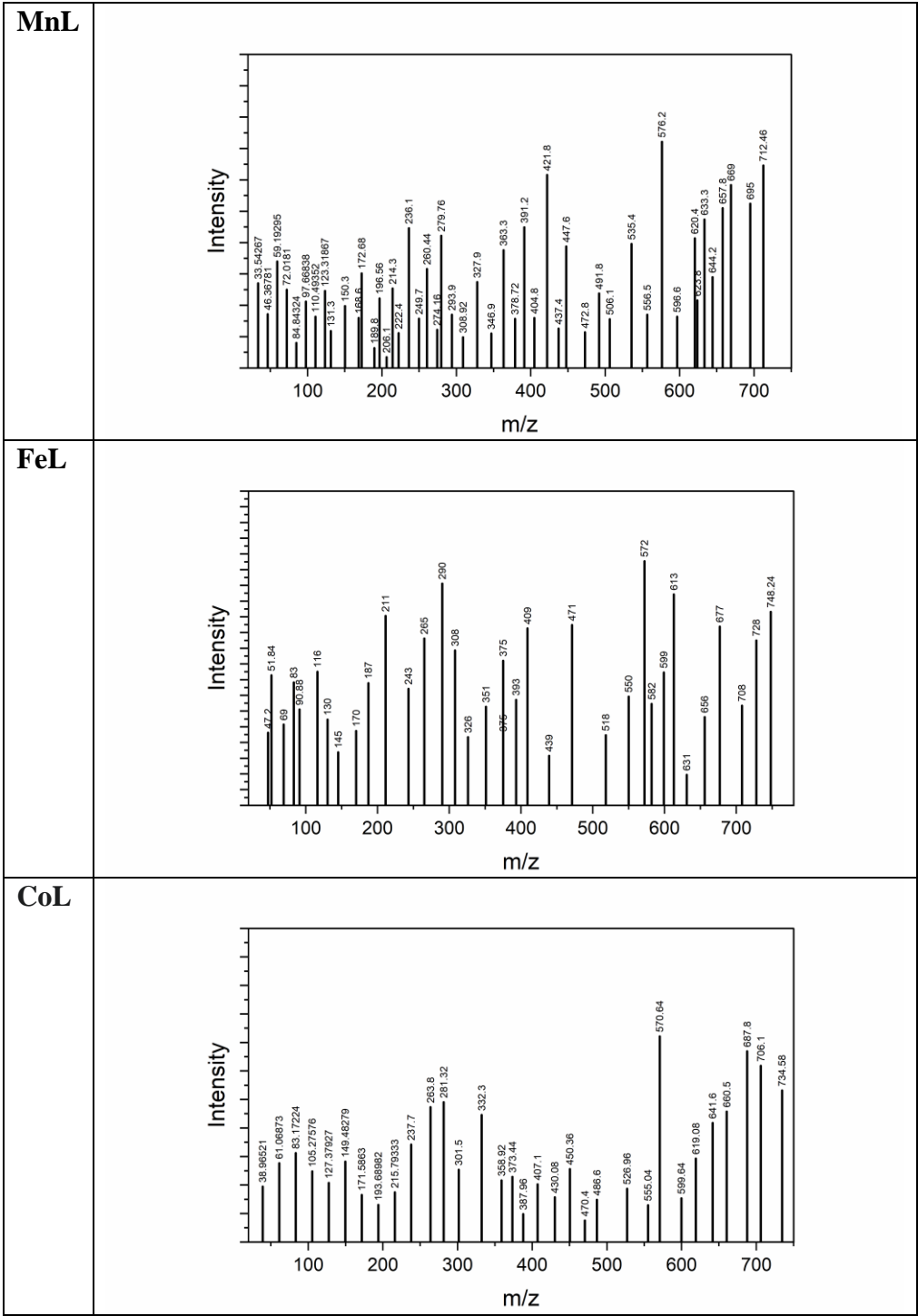
Figure S1: ^1H -NMR and ^{13}C -NMR of the azo-ligand (HL)

Figure S2: mass spectral of the subject complexes

Figure S3: The UV-vis. Spectra of the free ligand and its complexes.

Figure S4: Determination of composition of the metal complexes by jobs method of continuous variation method





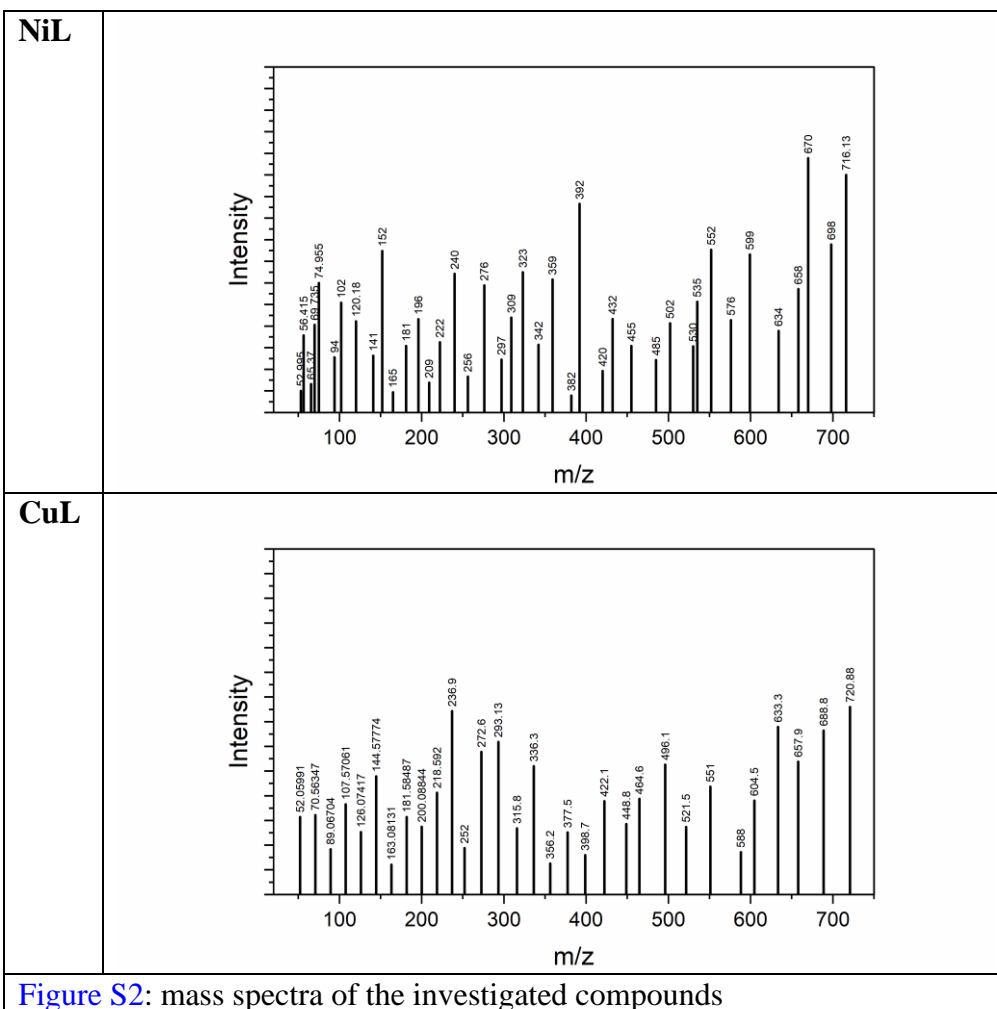


Figure S2: mass spectra of the investigated compounds

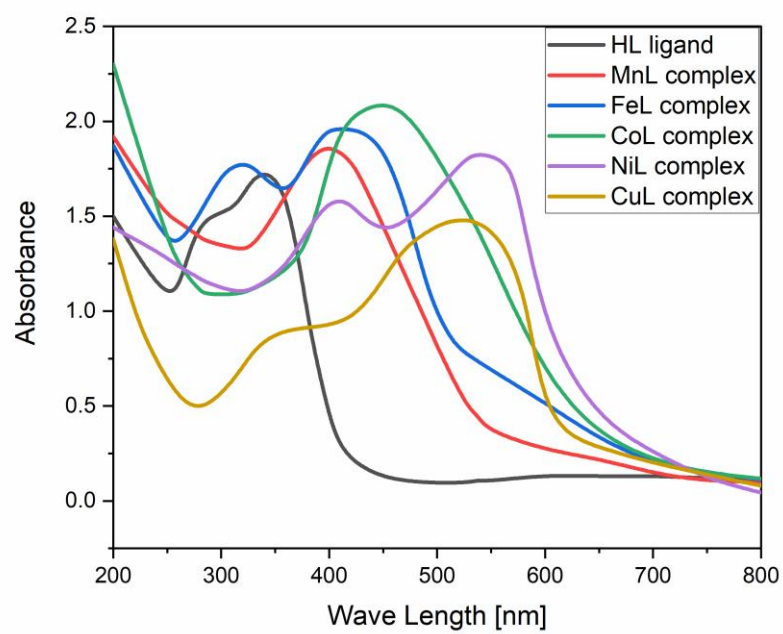


Figure S3: Electronic spectra

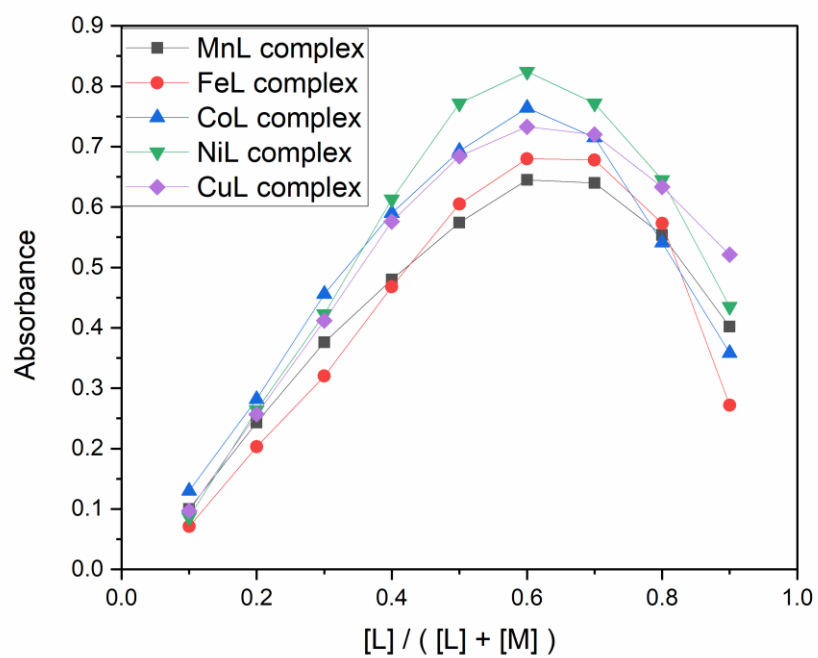


Figure S4: Determination of composition of the metal complexes by continuous variation method

Table S1: Comparison between the minimum inhibition concentration (MIC) of the current compounds with previously reported compounds in the literature survey against e. coli.

	E. coli (G⁻)	
		MIC
1	MnL [This work]	6.25
2	FeL [This work]	12.5
3	CoL [This work]	12.5
4	NiL [This work]	25
5	CuL [This work]	12.5
6	FeL [1]	50.00
7	CoL [1]	55.00
8	NiL [1]	60.00
9	CuL [1]	50.00
10	ZnL [1]	70.00
11	FeLQ [2]	25.50
12	FeLB [2]	22.50
13	FeLI [2]	23.50
14	CuLQ [3]	21.50
15	CuLB [3]	22.50
16	CuLI [3]	22.50
17	NiLQ [4]	35.50
18	NiLB [4]	34.50
19	NiLI [4]	37.50
20	complex M₅ [36]	25
21	[Zn(DIPO)Cl₂] [37]	80
22	[Co(DIPO)Cl₂] [37]	60
23	Na[Ni(L1)₃] [38]	< 20