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Synthesis, characterization, cytotoxic and antimicrobial activities of mixed-ligand hydrazone complexes of variable valence VO^{z+} ($z = 2, 3$)

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Electronic Supplementary Information

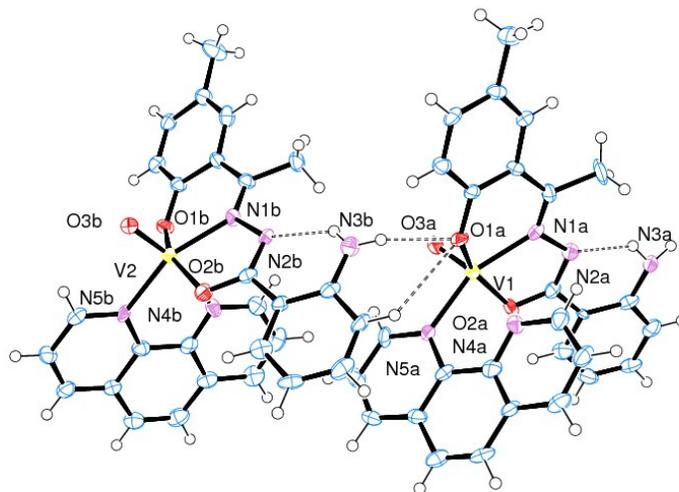


Fig. S1. Molecular structure of **2** with ellipsoids at 30% probability showing two molecules **A** and **B** are intermolecularly H-bonded. The hydrogen bonds are shown as dotted lines.

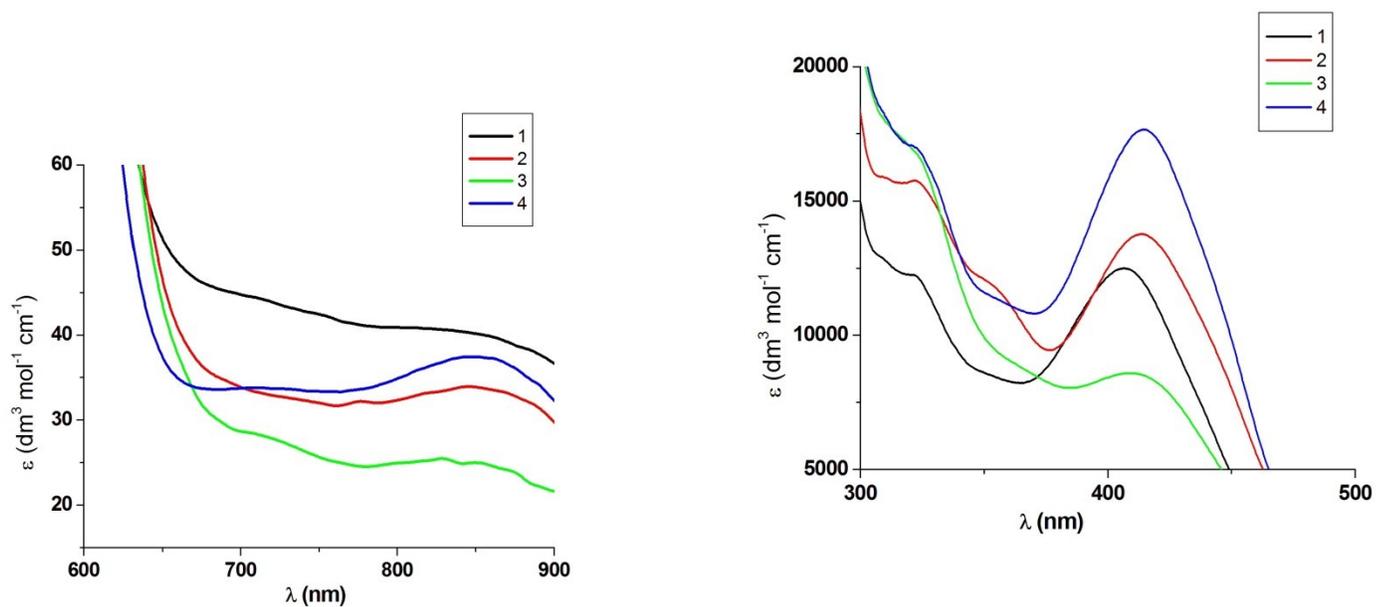


Fig. S2. Overlay of the electronic spectra of **1-4** complexes in CH_2Cl_2 solution.

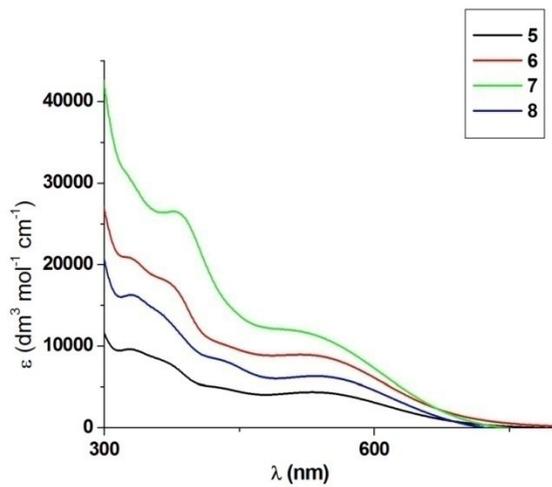
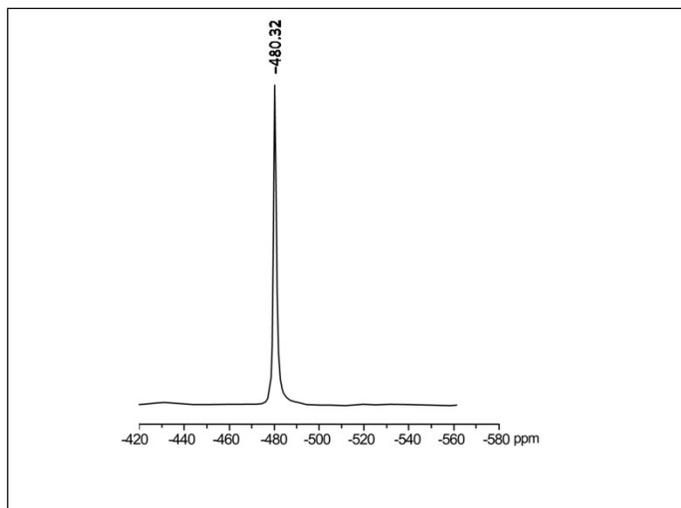
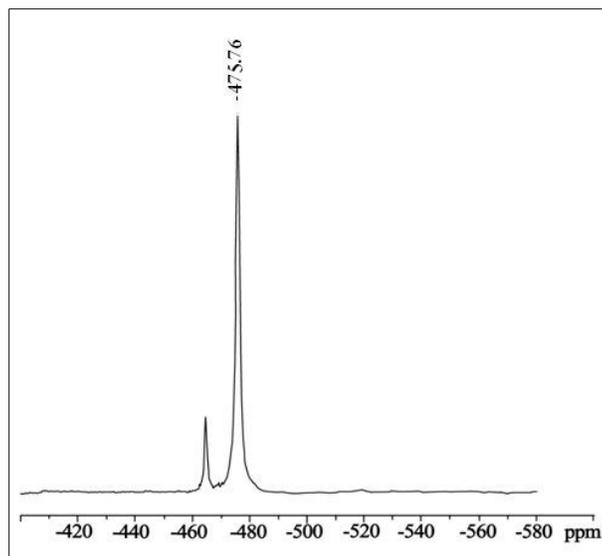


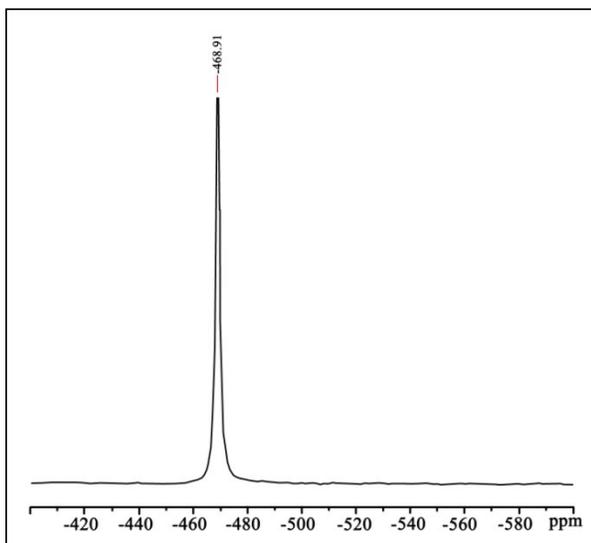
Fig. S3. Overlay of the electronic spectra of **5-8** complexes in CH_2Cl_2 solution.



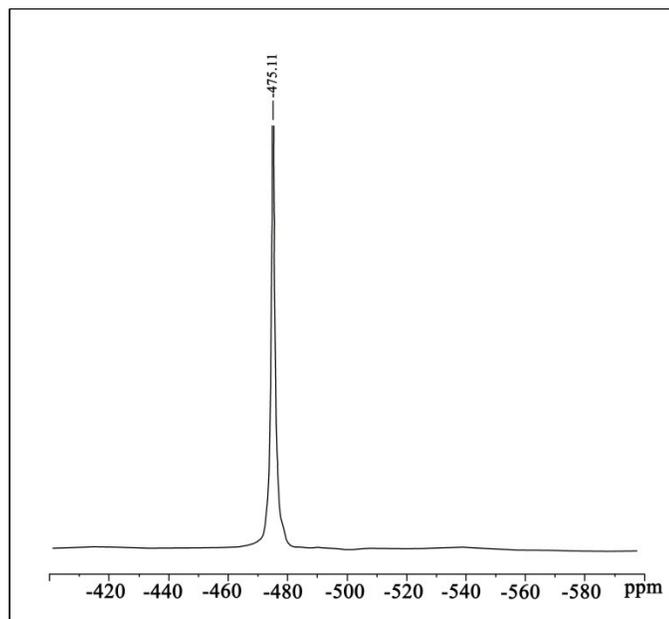
5



6



7



8

Fig. S4 ^{51}V NMR of complexes 5-8 in CDCl_3 solution at 298 K.

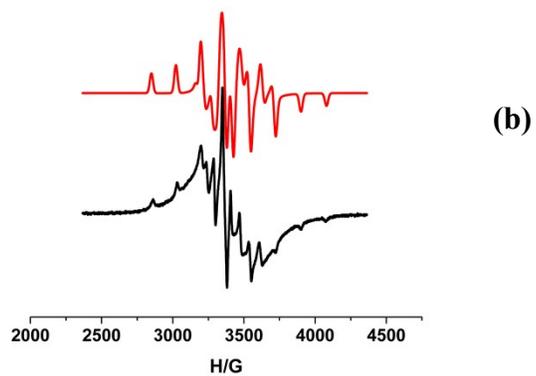
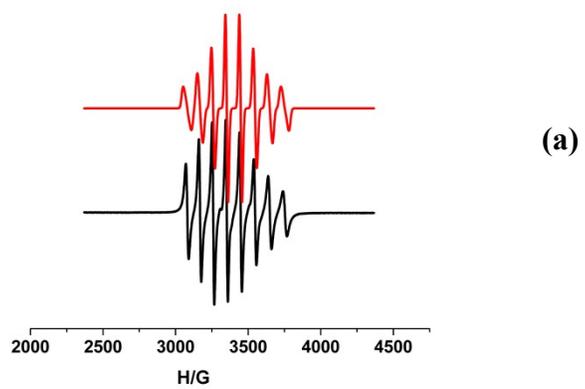


Fig. S5. X-band EPR spectra of complex **1** (black experimental; red simulated) in CH_2Cl_2 solution at 300 K (a) and at 77 K (b).

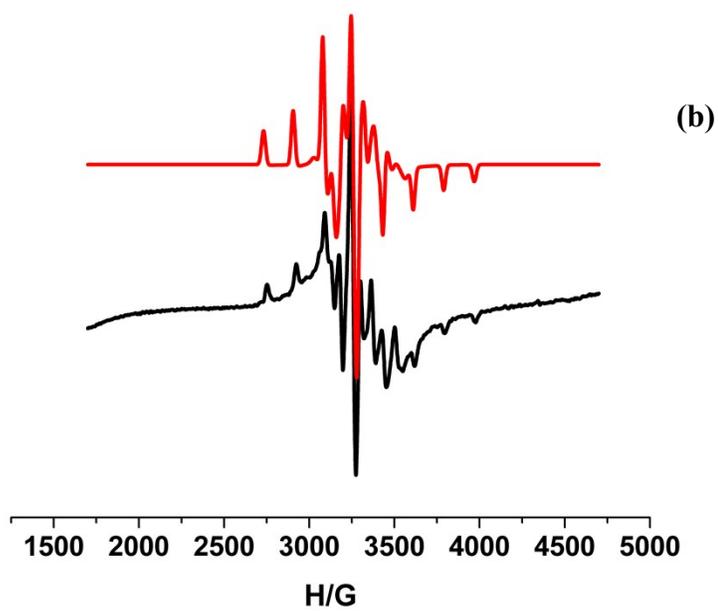
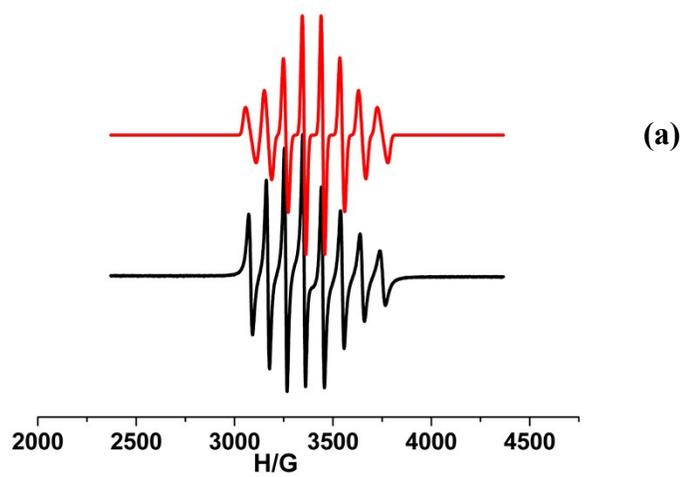


Fig. S6. X-band EPR spectra of complex **3** (black experimental; red simulated) in CH_2Cl_2 solution at 300 K (a) and at 77 K (b).

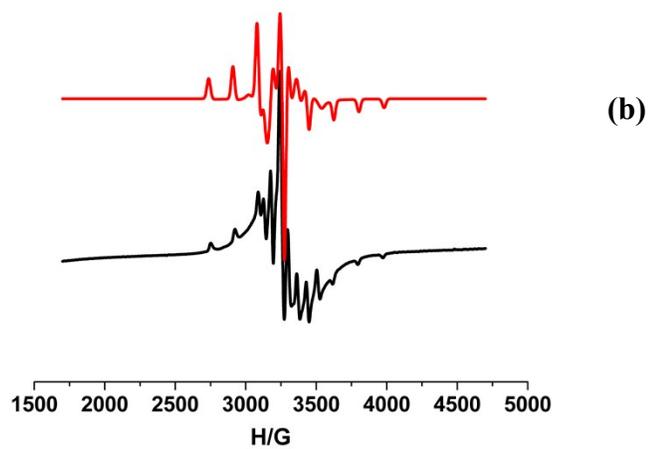
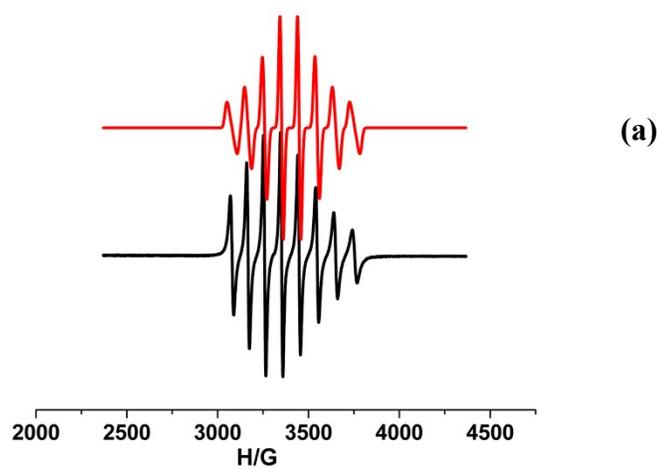


Fig. S7. X-band EPR spectra of complex **4** (black experimental; red simulated) in CH_2Cl_2 solution at 300 K (a) and at 77 K (b).

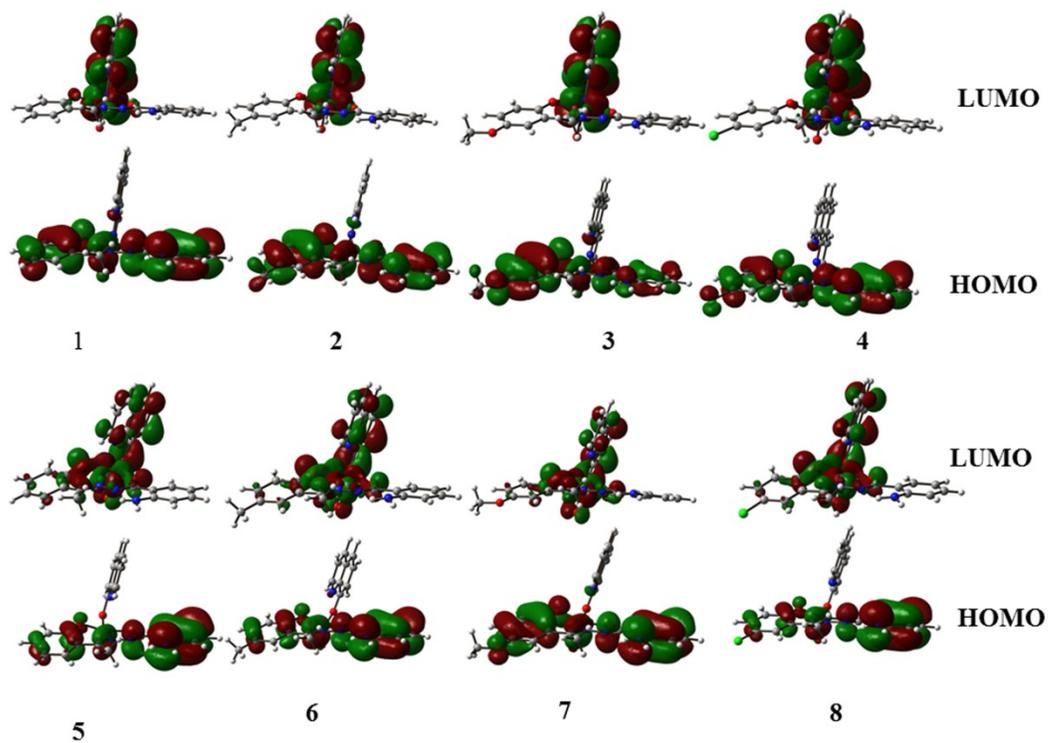


Fig. S8. Schematic diagram of selected frontier orbitals for complexes **1-8** in their ground state geometries.

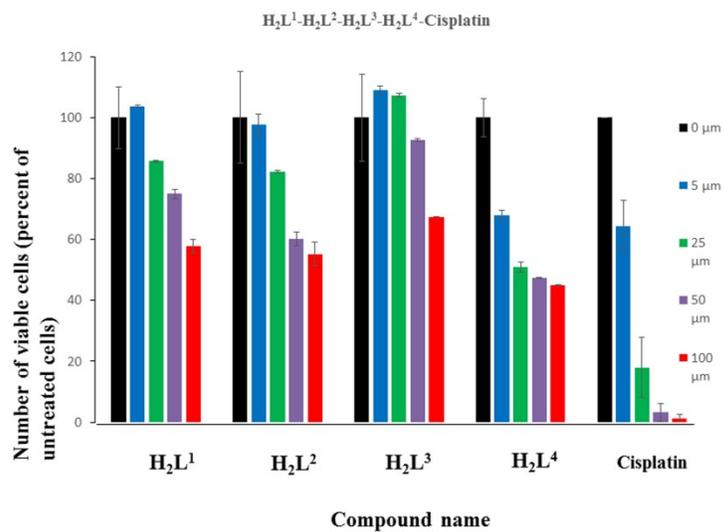


Fig. S9. Cytotoxic activity of the H_2L^{1-4} ligands.

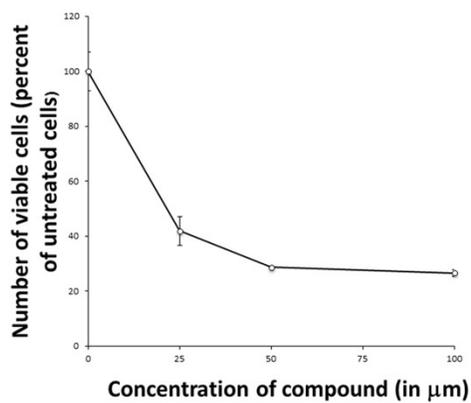


Fig. S10. Cytotoxic activity of $[V^{IV}O(aa)_2]$.

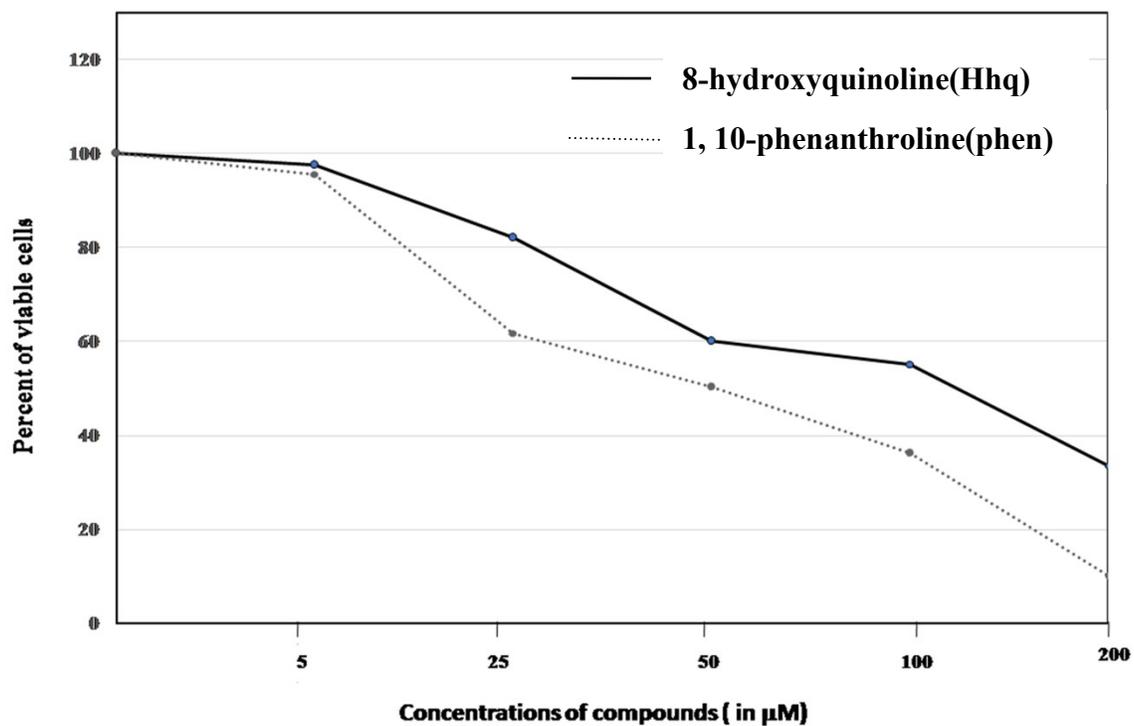
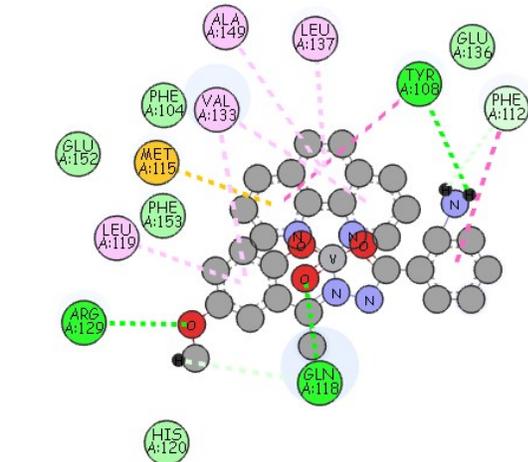
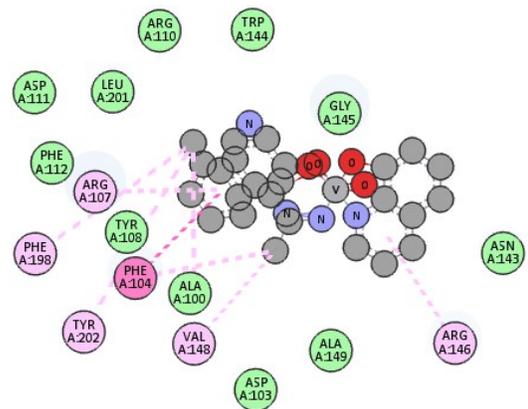


Fig. S11. Cytotoxic activity of 1,10-phenanthroline and 8-hydroxyquinoline.



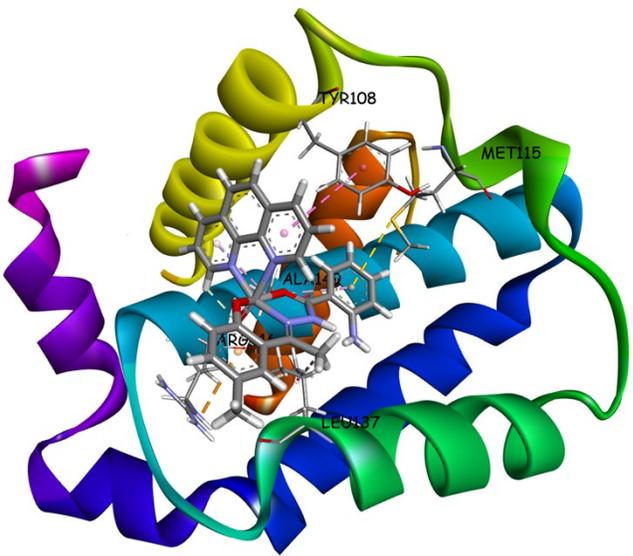
- Interactions**
- van der Waals
 - Conventional Hydrogen Bond
 - Carbon Hydrogen Bond
 - Pi-Donor Hydrogen Bond
 - Pi-Sulfur
 - Pi-Pi Stacked
 - Pi-Pi T-shaped
 - Pi-Alkyl

(a)

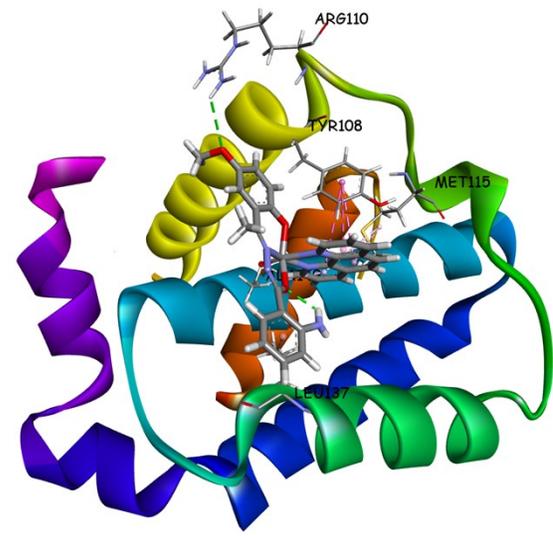


- Interactions**
- van der Waals
 - Pi-Pi T-shaped
 - Alkyl
 - Pi-Alkyl

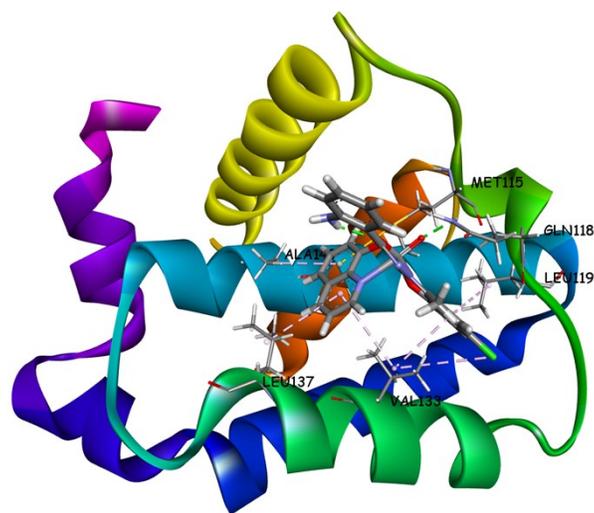
(b)



(c)



(d)



(e)

Fig S12: Two dimensional representation of binding site interacting with the molecules (a) **3** and (b) **6**. Docking pose of (c) compounds **2**, (d) compounds **3** and (e) compounds **8** with Bcl2 protein.

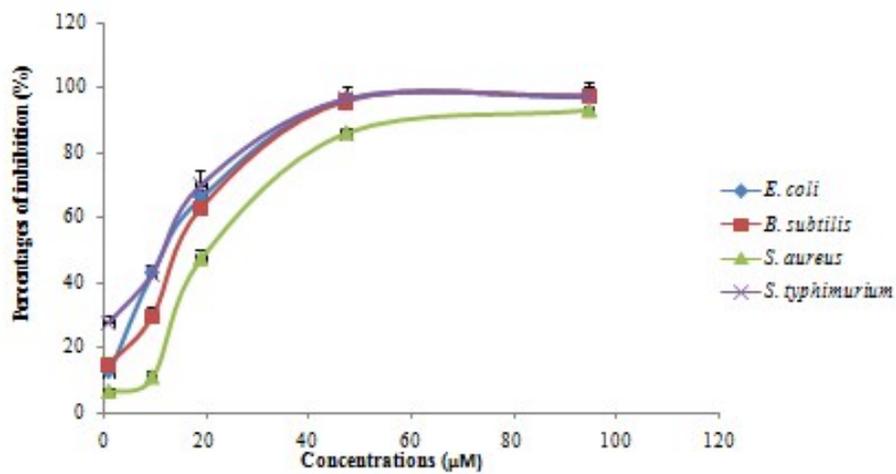


Fig. S13. Dose response curve for antimicrobial activity by complex **2**.

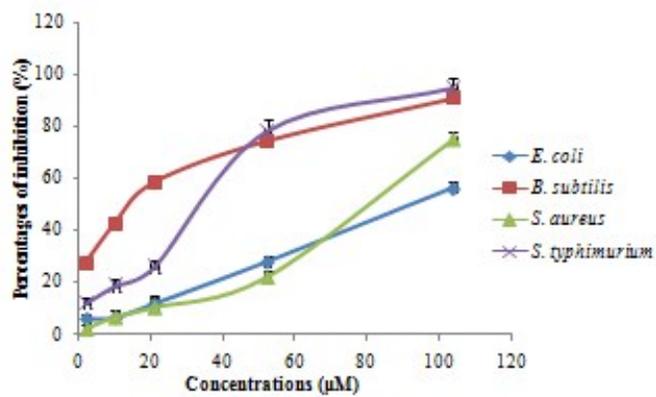


Fig. S14. Dose response curve for antimicrobial activity by complex 5.

Table S1. Calculated geometrical parameters for **1**, **2**, **3** and **4** complexes.

Complex	1	2	3	4
Bond lengths, Å				
V-O1	1.929	1.927	1.922	1.934
V-O2	1.987	1.989	1.993	1.986
V-O3	1.601	1.602	1.601	1.599
V-N4	2.197	2.199	2.198	2.195
V-N5	2.435	2.435	2.436	2.429
V-N1	2.067	2.065	2.069	2.071
Bond angles, degrees				
O3-V-O2	102.94	103.09	103.01	103.21
O3-V-O1	103.42	103.50	103.01	103.21
O3-V-N4	92.39	92.43	92.45	92.28
O3-V-N5	163.59	163.55	163.57	163.55
O3-V-N1	104.87	104.69	104.56	104.58
O2-V-N4	93.71	93.52	93.59	93.97
O2-V-N5	78.47	78.26	78.07	78.47
O2-V-N1	77.09	77.08	76.94	77.01
O1-V-O2	151.55	151.75	151.36	151.53
O1-V-N4	95.16	95.29	95.33	95.27
O1-V-N5	79.14	79.13	79.21	79.15
O1-V-N1	86.48	86.55	86.56	86.36
N5-V-N4	71.16	71.13	71.13	71.28
N1-V-N4	161.81	169.89	161.94	162.25
N1-V-N5	91.44	91.63	91.69	91.79

Table S2. Calculated geometrical parameters for complexes **5**, **6**, **7** and **8**.

Complex	5	6	7	8
Bond lengths, Å				
V-O1	1.843	1.840	1.835	1.848
V-O2	1.928	1.930	1.933	1.925
V-O3	1.582	1.582	1.583	1.581
V-O4	1.839	1.839	1.839	1.835
V-N1	2.116	2.116	2.122	2.121
V-N4	2.491	2.492	2.492	2.487
Bond angles, degree				
O3-V-O1	100.82	100.84	101.05	100.71
O3-V-O4	102.73	102.73	102.69	102.72
O1-V-O4	102.09	102.14	102.37	101.85
O3-V-O2	101.85	101.85	101.75	101.95
O1-V-O2	149.80	149.82	149.54	149.72
O4-V-O2	92.07	91.97	92.01	92.46
O3-V-N1	96.99	97.03	96.75	96.86
O1-V-N1	82.79	82.83	82.78	82.75
O4-V-N1	158.27	158.20	158.40	158.57
O2-V-N1	74.88	74.89	74.74	74.86
O3-V-N4	176.78	176.75	176.69	176.88
O1-V-N4	80.26	80.38	80.45	80.24
O4-V-N4	74.05	74.04	74.07	74.17
O2-V-N4	78.20	78.06	77.89	78.20
N1-V-N4	86.13	86.08	86.33	86.19

Table S3. IC₅₀ values on lung cancer cell line and binding energies of complexes **1-8** with Bcl2 protein.

Complex	IC ₅₀ (μM)	Binding energy (ΔG in kcal/mol) ± SD
1	7.5	-7.15 ± 0.21
2	2.5	-7.39 ± 0.23
3	2.5	-7.46 ± 0.11
4	2.5	-7.41 ± 0.42
5	12.5	-6.86 ± 0.15
6	5	-7.08 ± 0.24
7	25	-6.63 ± 0.35
8	5	-6.95 ± 0.29