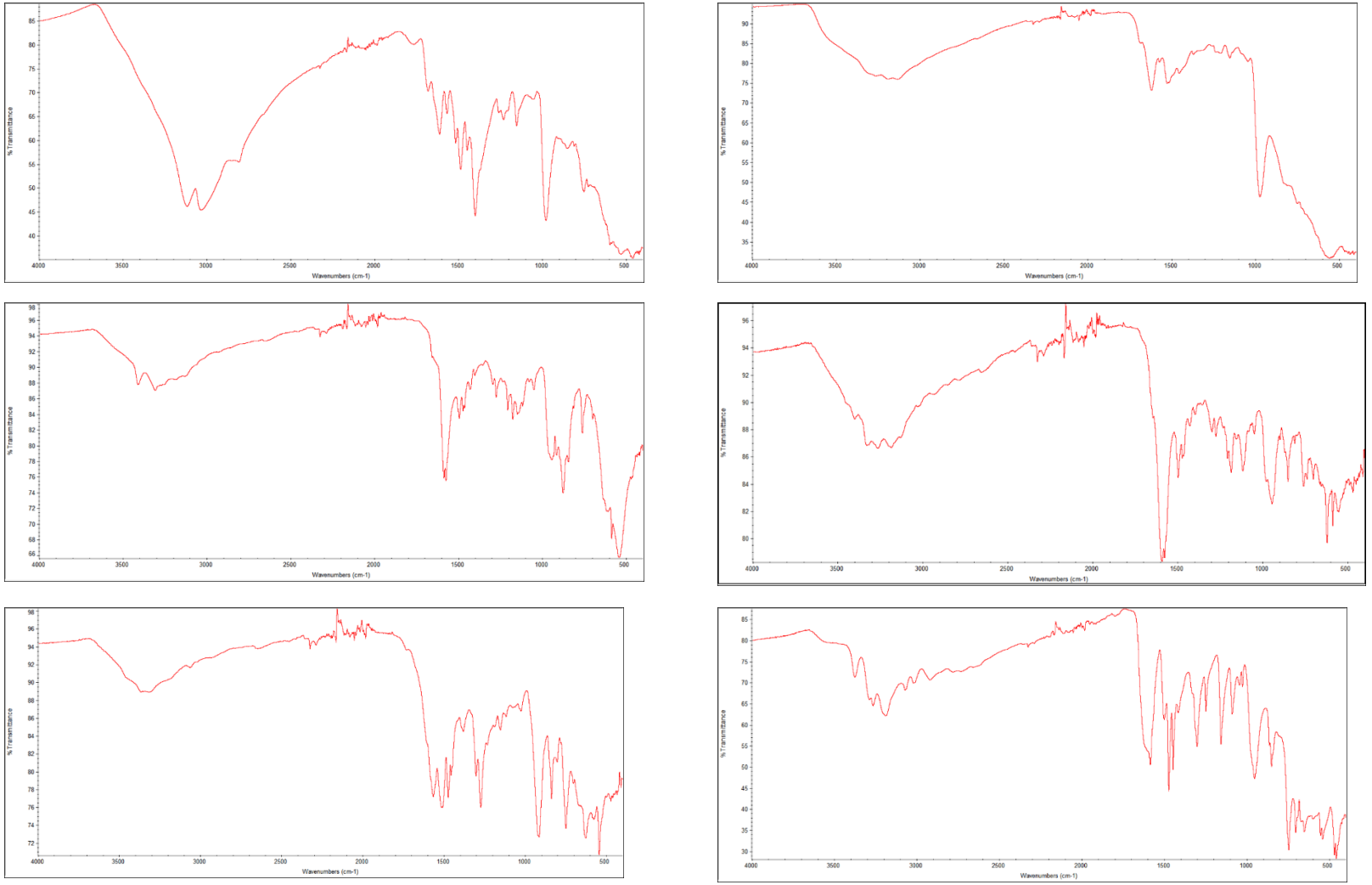

Fig. S1. IR spectrum for **(1-6)** complexes.

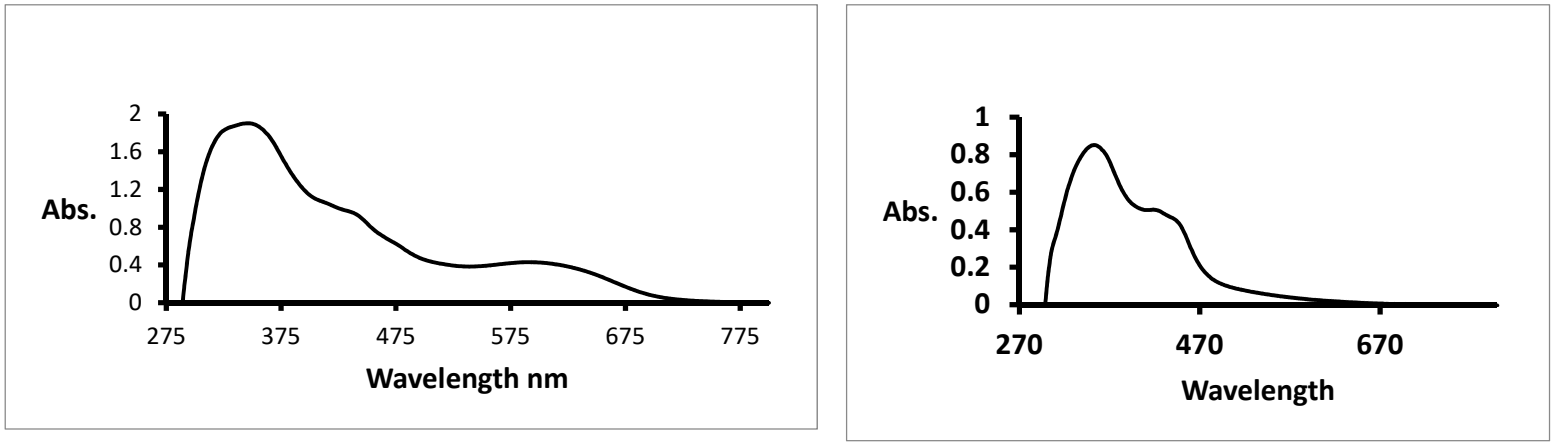

Fig. S2. The electronic spectrum of **(1 and 4)** complex.

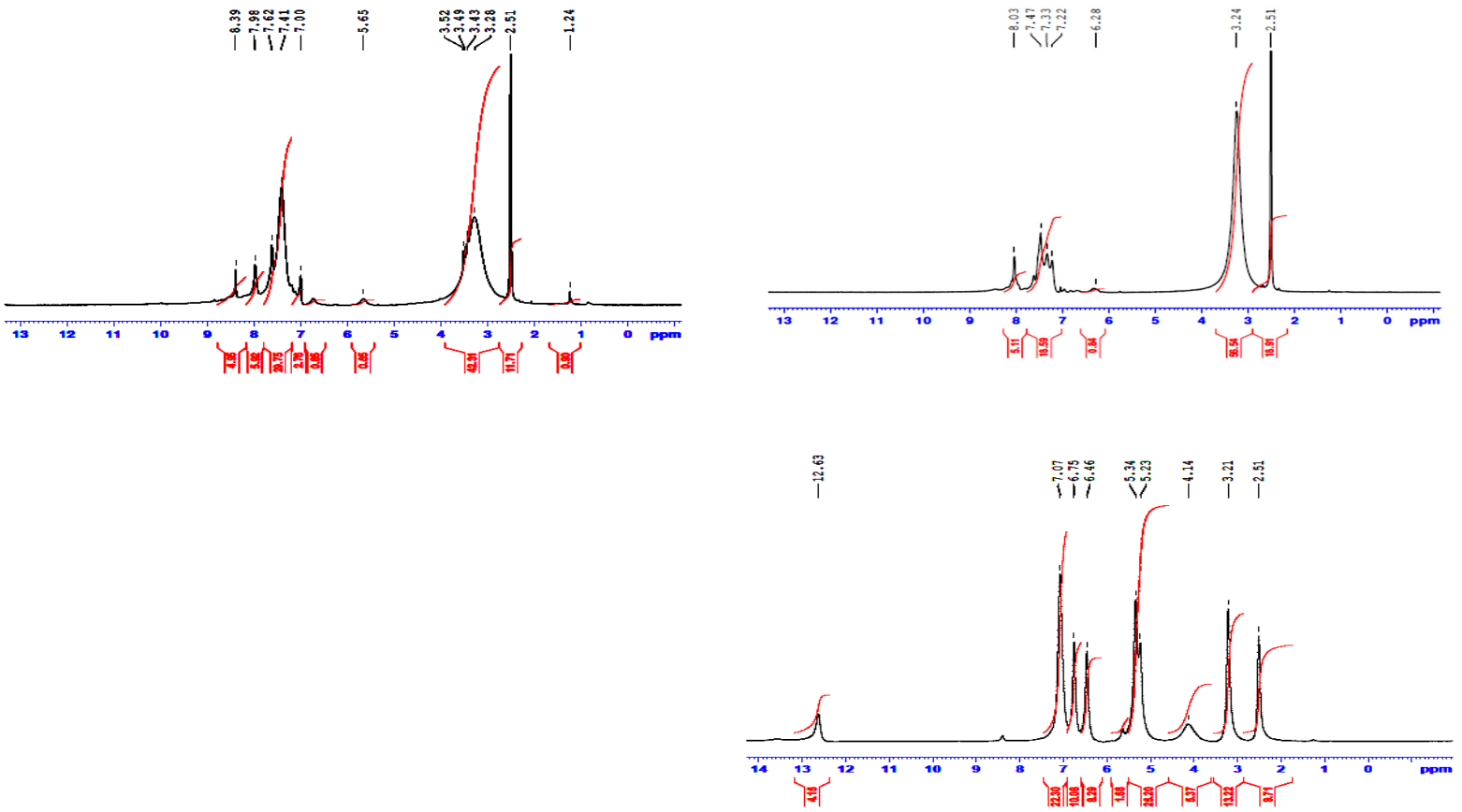

Figure S3: ^{1}H NMR spectrum of complexes (1-3).

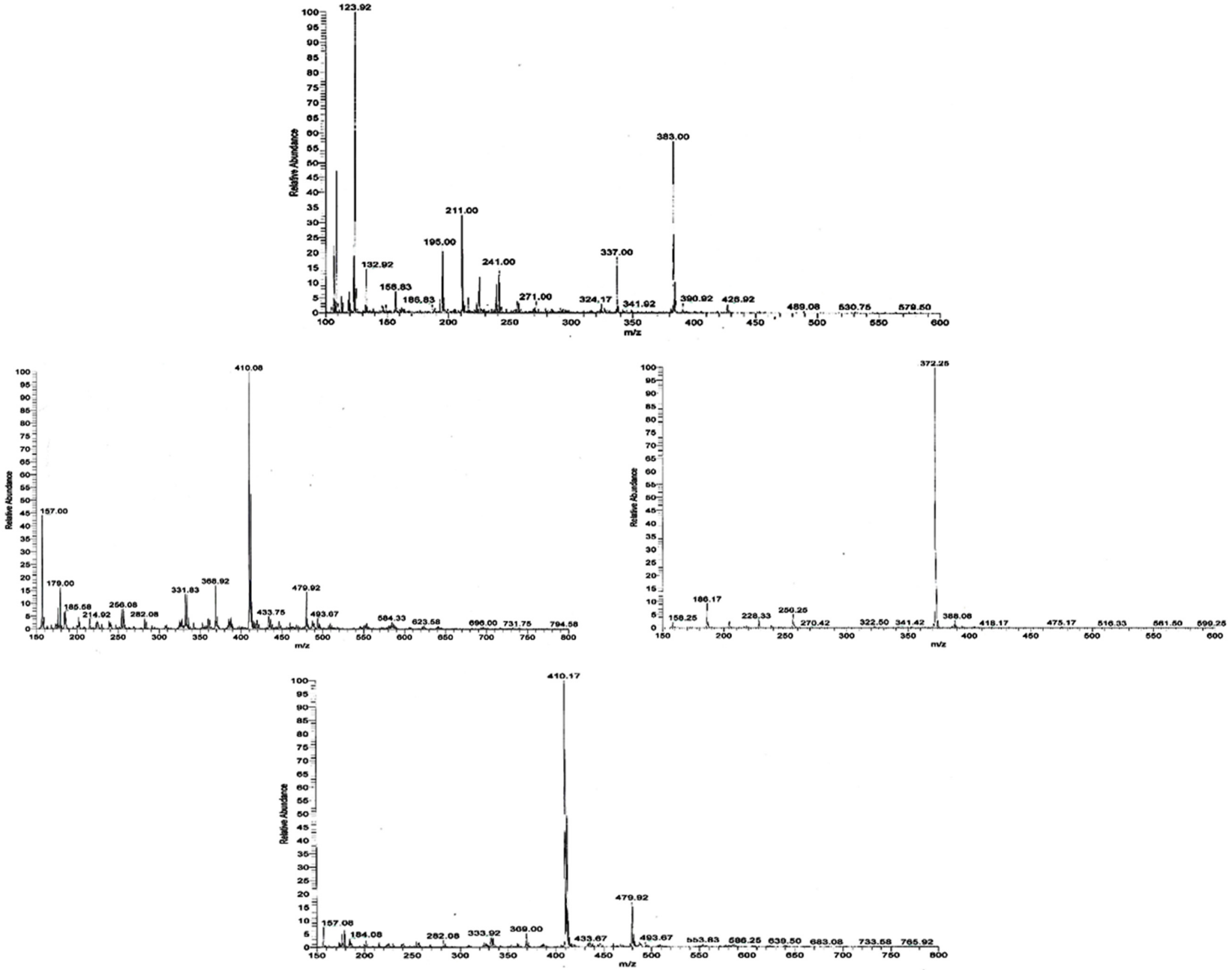

Figure S.4: Mass spectra for **(1,3,5,6)** complexes.

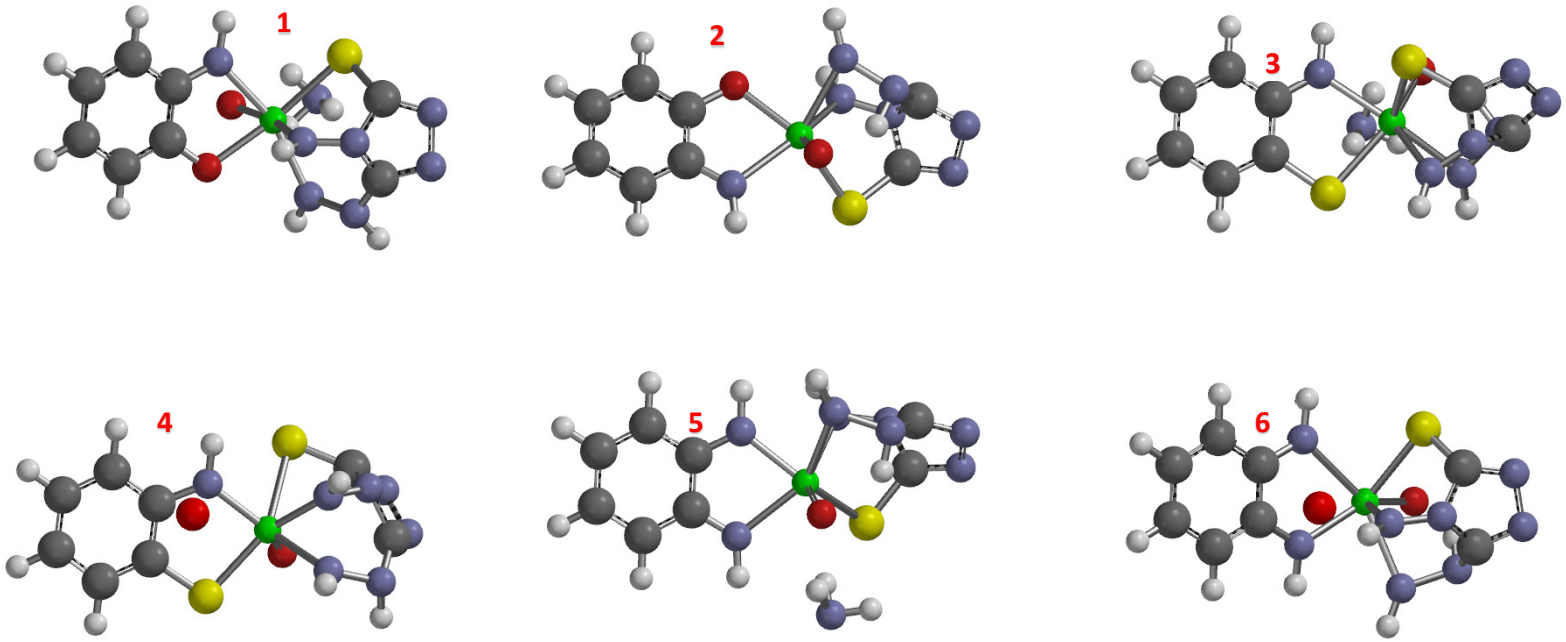

Figure S5: optimization geometry of tested complexes (**1-6**) at DFT/ B3LYP/6-311G++(d,p).

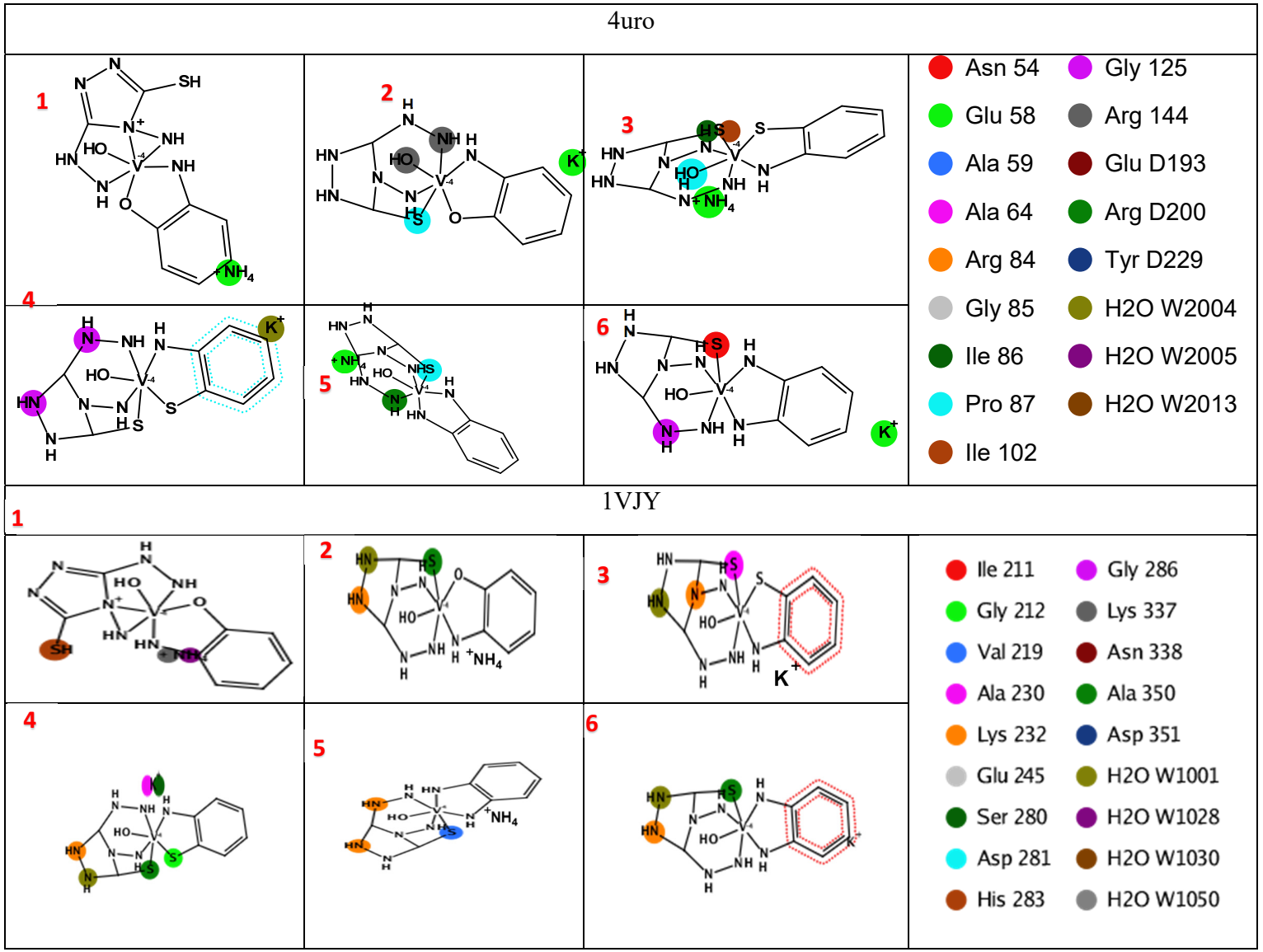

Figure S. 6: Schematic interactions between ligands and proteins 4uro and 1VJY using protein-ligand interaction fingerprint tools.

Table S 1: The elemental analysis data and molar conductance measurements of the Vanadium (V) Complexes.

Compound	Mol. Formula	Yield	Mol. Wt.	Cald(Found)%					Molar conductance
				C	H	N	O	S	(ohm-1 cm2 mol-1)
NH4[VO(L1)(L2)]2.5H2O (1)	C8H22N9SO3.5V	80%	383.3	25.07 (25.25)	5.79 (5.93)	32.90 (32.73)	14.57 (14.26)	8.36 (8.52)	110.5
K[VO(L1)(L2)]1.5H2O (2)	C8H16N8SO2.5VK	78%	386.35	24.87 (24.96)	4.17 (4.34)	29.01 (29.35)	10.31 (10.52)	8.30 (8.45)	95.3
NH4[VO(L1)(L3)]H2O (3)	C8H22N8SO6V	85%	409.29	23.47 (23.64)	5.42 (5.53)	27.38 (27.56)	23.45 (23.72)	7.83 (7.96)	85.8
K[VO(L1)(L3)] H2O (4)	C8H13N7SO3VK	79%	377.32	25.46 (25.73)	3.47 (3.58)	25.98 (26.24)	12.72 (12.85)	8.50 (8.67)	93.2
NH4[VO(L1)(L4)]H2O (5)	C8H17N8S2O2V	75%	372.32	25.81 (25.98)	4.60 (4.72)	30.09 (30.25)	8.59 (8.69)	17.22 (17.35)	79.2
K[VO(L1)(L4)]2 H2O (6)	C8H15N7S2O3VK	70%	411.39	23.35 (23.45)	3.67 (3.82)	23.83 (23.95)	11.67	15.59 15.76)	75.6

Table S2: IR Spectroscopic data (cm-1) of the ligands and their vanadium (V) complexes.

Compound	NH2 and H2O	SH	V=O	V-S	V-N	V-O
L1	3270, 3200	2910	-	-		-
NH4[VO(L1)(L2)] 2.5H2O (1)	3110 3050	-	980	450	540	-
K[VO(L1)(L2)] 1.5H2O (2)	3280 3200	-	980	470	550	-
NH4[VO(L1)(L3)] 4H2O (3)	3405 3300	-	950	480	540	595
K[VO(L1)(L3)] H2O (4)	3290 3330	-	960	450	535	590
NH4[VO(L1)(L4)] H2O (5)	3310 339	-	920	470	550	-
K[VO(L1)(L4)]2 H2O (6)	3300 3380	-	980	450	530	-

Table S3: bond length and angles for complexes **1-6.**

Atom		°	Atom	A°	Atom		°	Atom	A°	Atom		°	Atom	A°	Atom		°	Atom	A°
		1					2					3					4		
C(2)	N(1)	1.374			C(2)	N(1)	1.323			C(2)	N(1)	1.322	C(2)	104.747	C(2)	N(1)	1.355		
N(3)	N(1)	1.339	C(2)	110.493	N(3)	N(1)	1.399	C(2)	104.753	N(3)	N(1)	1.398	N(1)	107.29	N(3)	N(1)	1.369	C(2)	109.589
N(4)	C(2)	1.418	N(1)	104.652	N(4)	C(2)	1.383	N(1)	107.186	N(4)	C(2)	1.38	N(1)	128.106	N(4)	C(2)	1.476	N(1)	107.237
S(6)	C(2)	1.72	N(1)	132.03	S(6)	C(2)	1.774	N(1)	127.964	S(6)	C(2)	1.77	N(1)	105.001	S(6)	C(2)	1.712	N(1)	134.145
C(5)	N(3)	1.362	N(1)	108.48	C(5)	N(3)	1.335	N(1)	104.978	C(5)	N(3)	1.335	N(3)	126.934	C(5)	N(3)	1.36	N(1)	108.346
N(7)	C(5)	1.435	N(3)	132.507	N(7)	C(5)	1.385	N(3)	126.954	N(7)	C(5)	1.384	C(2)	119.106	N(7)	C(5)	1.442	N(3)	135.139
N(8)	N(4)	1.473	C(2)	122.842	N(8)	N(4)	1.337	C(2)	119.098	N(8)	N(4)	1.337	C(5)	116.422	N(8)	N(4)	1.406	C(2)	116.755
N(9)	N(7)	1.498	C(5)	101.972	N(9)	N(7)	1.526	C(5)	116.427	N(9)	N(7)	1.525	C(2)	96.001	N(9)	N(7)	1.445	C(5)	104.645
H(21)	N(7)	0.997	C(5)	110.849	V(18)	S(6)	2.491	C(2)	95.23	V(18)	S(6)	2.5	S(6)	86.912	V(18)	S(6)	2.556	C(2)	81.922
V(18)	S(6)	2.573	C(2)	71.929	N(16)	V(18)	2.209	S(6)	95.059	N(16)	V(18)	2.237	S(6)	126.561	N(16)	V(18)	1.999	S(6)	77.637
N(16)	V(18)	2.049	S(6)	71.569	O(17)	V(18)	2.135	S(6)	137.84	S(17)	V(18)	2.441	S(6)	90.62	S(17)	V(18)	2.317	S(6)	144.738
O(17)	V(18)	1.992	S(6)	82.467	O(19)	V(18)	1.909	S(6)	95.72	O(19)	V(18)	1.909	V(18)	97.572	O(19)	V(18)	1.592	S(6)	82.371
N(20)	V(18)	2.061	S(6)	82.865	C(12)	O(17)	1.366	V(18)	111.878	C(12)	S(17)	1.779	S(17)	118.962	C(12)	S(17)	1.732	V(18)	99.515
O(19)	V(18)	1.66	S(6)	156.041	C(10)	C(12)	1.393	O(17)	119.149	C(10)	C(12)	1.403	V(18)	117.586	C(10)	C(12)	1.392	S(17)	121.662
C(12)	O(17)	1.296	V(18)	112.831	C(14)	N(16)	1.335	V(18)	111.42	C(14)	N(16)	1.341	C(12)	119.944	C(14)	N(16)	1.39	V(18)	121.162
C(10)	C(12)	1.425	O(17)	122.439	C(15)	C(14)	1.399	C(12)	120.106	C(15)	C(14)	1.405	C(12)	120.719	C(15)	C(14)	1.416	C(12)	119.069
C(14)	N(16)	1.364	V(18)	112.062	C(11)	C(10)	1.398	C(12)	119.699	C(11)	C(10)	1.398	C(11)	119.611	C(11)	C(10)	1.399	C(12)	119.797
C(15)	C(14)	1.417	C(12)	120.452	C(13)	C(15)	1.398	C(14)	119.7	H(24)	C(10)	1.086	C(14)	120.457	C(13)	C(15)	1.394	C(14)	119.426
C(11)	C(10)	1.375	C(12)	119.742						C(13)	C(15)	1.396							
C(13)	C(15)	1.376	C(14)	119.361															
5							**6**												
C(2)	N(1)	1.321			C(2)	N(1)	1.32												
N(3)	N(1)	1.396	C(2)	104.831	N(3)	N(1)	1.393	C(2)	104.858										
N(4)	C(2)	1.382	N(1)	107.548	N(4)	C(2)	1.38	N(1)	107.443										
S(6)	C(2)	1.769	N(1)	128.111	S(6)	C(2)	1.763	N(1)	127.538										
C(5)	N(3)	1.335	N(1)	105.113	C(5)	N(3)	1.332	N(1)	105.088										
N(7)	C(5)	1.385	N(3)	126.703	N(7)	C(5)	1.38	N(3)	126.49										
N(8)	N(4)	1.334	C(2)	118.653	N(8)	N(4)	1.339	C(2)	119.747										
N(9)	N(7)	1.523	C(5)	116.423	N(9)	N(7)	1.51	C(5)	116.294										
V(18)	S(6)	2.491	C(2)	95.056	V(18)	S(6)	2.511	C(2)	97.016										
N(16)	V(18)	2.226	S(6)	102.754	N(16)	V(18)	2.356	S(6)	78.133										
N(17)	V(18)	2.095	S(6)	135.829	N(17)	V(18)	2.064	S(6)	141.658										
O(19)	V(18)	1.909	S(6)	106.207	O(19)	V(18)	1.917	S(6)	82.361										
C(12)	N(17)	1.339	V(18)	115.07	C(12)	N(17)	1.34	V(18)	118.302										
C(10)	C(12)	1.395	N(17)	120.874	C(10)	C(12)	1.394	N(17)	120.605										
C(14)	N(16)	1.333	V(18)	111.417	C(14)	N(16)	1.338	V(18)	108.965										
C(15)	C(14)	1.4	C(12)	120.526	C(15)	C(14)	1.399	C(12)	120.536										
C(11)	C(10)	1.398	C(12)	119.948	C(11)	C(10)	1.398	C(12)	119.819										
C(13)	C(15)	1.398	C(14)	119.644	C(13)	C(15)	1.397	C(14)	119.517										
N(20)	C(13)	6.629	C(11)	112.142															

Table S4: Docking energy scores (kcal/mol) derived from the MOE for investigated complexes 1-6 and reference inhibitors Novobiocin & Naphthyridine

ΔG	**E_H.B**	**rmsd**	**E_Int**	**Evdw**	**E_Ele.**
PDB ID: 4uro					

1	-4.48689	±	0.40146	-19.1809	4.858089	-13.5443	±	1.181913	-12.7061	±	1.965668	-687.076
2	-3.29417	±	0.313169	-3.2513	8.880264	-14.1657	±	1.125484	-15.8495	±	2.180657	-1319.36
3	-2.99625	±	5.485056	5.744313	3.335386	-16.4849	±	0.709926	-14.769	±	4.565245	-1406.31
4	-3.77885	±	0.502814	-8.28987	4.481207	-15.6308	±	1.09749	-15.1112	±	1.690113	-1385.86
5	-3.09643	±	0.32078	-1.12529	6.064763	-16.2199	±	0.531064	-9.92016	±	2.013327	-1553.17
6	-3.01162	±	0.957208	17.07411	1.859781	-15.0097	±	1.305734	-17.9566	±	3.085084	-1535.74
Nov.	-7.88632	±	0.914276	-14.7029	1.85983	-42.9322	±	1.1120143	-15.6593	±	1.36589	-63.2072
PDB ID: 1VJY												
1	-3.73004	±	1.11201	-14.317	2.430106	-9.1911	±	0.91428	12.74759	±	2.80534	-665.783
2	-2.38761	±	1.04971	-16.7793	2.787305	-11.1083	±	0.89209	100.7158	±	2.86877	-1281.68
3	-2.9139	±	0.9874	-16.5177	2.396107	-5.86862	±	0.8699	48.14878	±	2.9322	-1399.13
4	-2.25492	±	0.9251	-17.2917	2.679346	-8.56476	±	0.84771	102.8958	±	2.99563	-1333.25
5	-5.0434	±	0.86279	-18.3904	1.318259	-9.9844	±	0.82552	-31.7604	±	3.05905	-1508.34
6	-4.128591	±	0.80049	-14.7752	1.370579	-13.358	±	0.80333	131.5203	±	3.12248	-1499.33
Nap.	-6.4348282	±	0.06951	-12.4992	1.492011	-27.236	±	0.70365	44.6523	±	1.25634	-106.36

ΔG.: Free binding energy of the ligand from a given conformer, Int.: Affinity binding energy of hydrogen bond interaction with receptor, H.B.: Hydrogen bonding energy between protein and ligand. Eele: Electrostatic interaction with the receptor, Evdw: Van der Waals energies between the ligand and the receptor.