Fluorescence Quenching of V(III) Ion by 4-Benzylaniline allied Schiff Base Functionalized Organosilane: unveiling antiproliferative Potential through In Vitro Analysis and Molecular Docking

Gurjaspreet Singh[a*], Jyoti[a*], Amanpreet Singh[b], Devina Sharma[a], Baljinder Singh Gill[c], Jandeep Singh[d], Nancy George[d], Deepanjali Baliyan[c], Amarjit Kaur[a]

[a]*Department of chemistry, Panjab University, Chandigarh, 160014, India*

[b]*RAYAT-BAHRA Group of Institutes, Chemistry*

[c]*Department of Biochemistry, Central University of Punjab, Bathinda, 151401, India*

[d]*School of Chemical Engineering and Physical Sciences, Lovely Professional University, Phagwara, Punjab 144411, India*

[*]Corresponding Authors

1. Prof. Gurjaspreet Singh

Department of Chemistry & Centre of Advanced Studies

Panjab University, Chandigarh, India

Email: gjpsingh@pu.ac.in

2. Mrs. Jyoti

Research Scholar

Department of Chemistry & Centre of Advanced Studies

Panjab University, Chandigarh, India

Email: jyotinain66@gmail.com

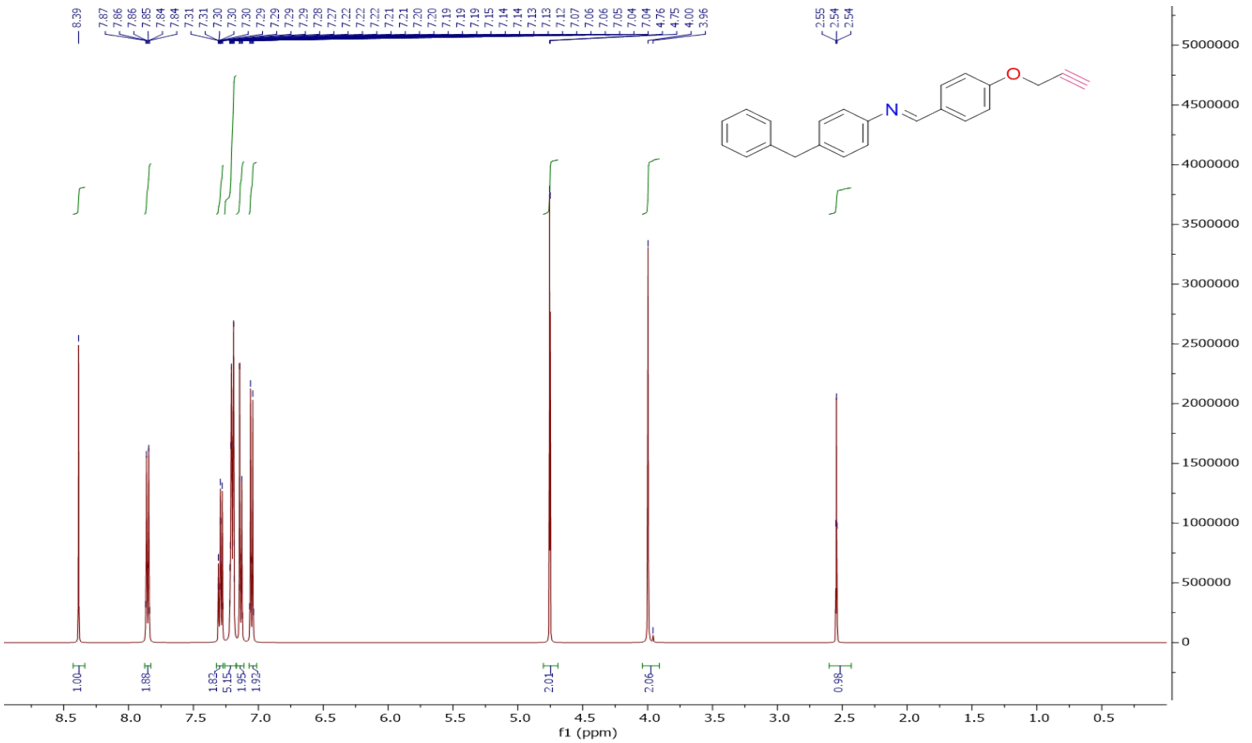

Fig. S1. ^{1}H NMR Spectra of compound 4

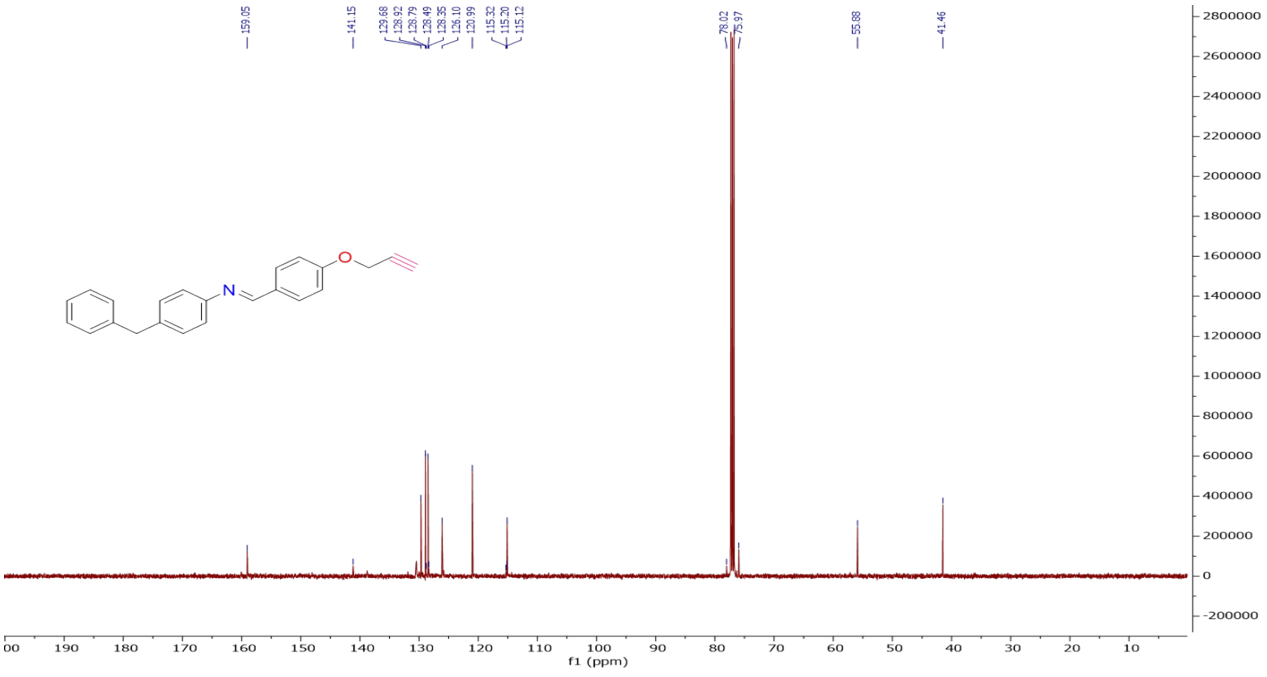

Fig. S2. ^{13}C NMR Spectra of compound 4

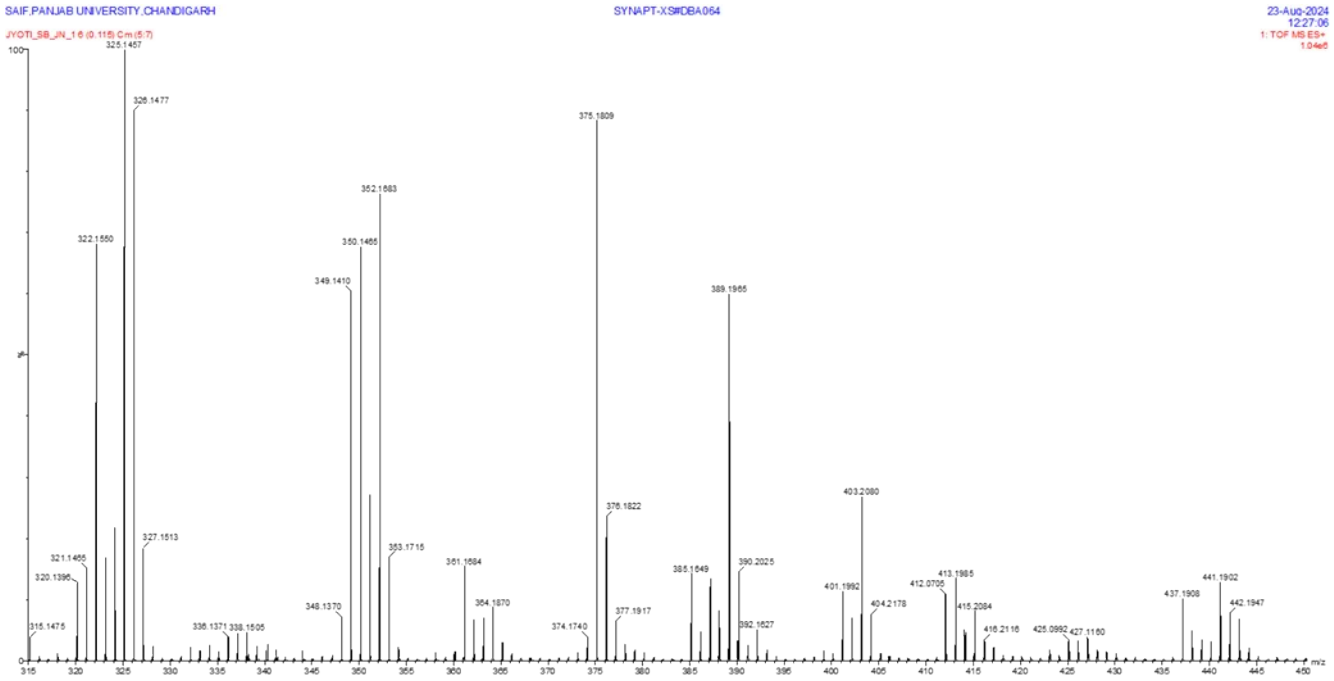

Fig. S3. Mass Spectra of compound 4

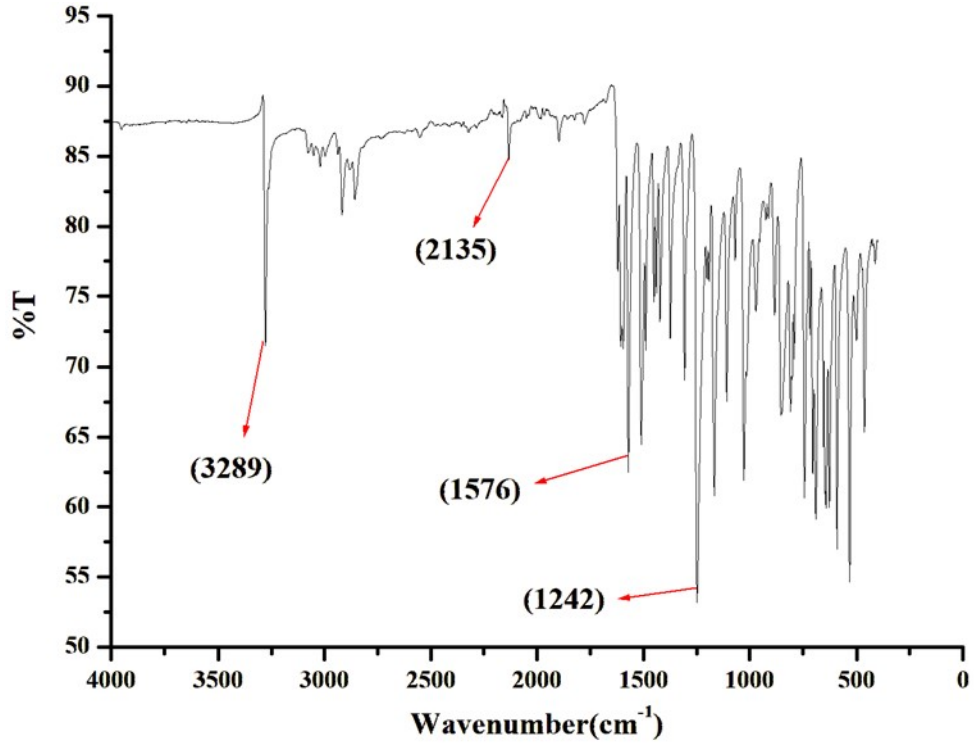

Fig. S4. IR Spectra of compound 4

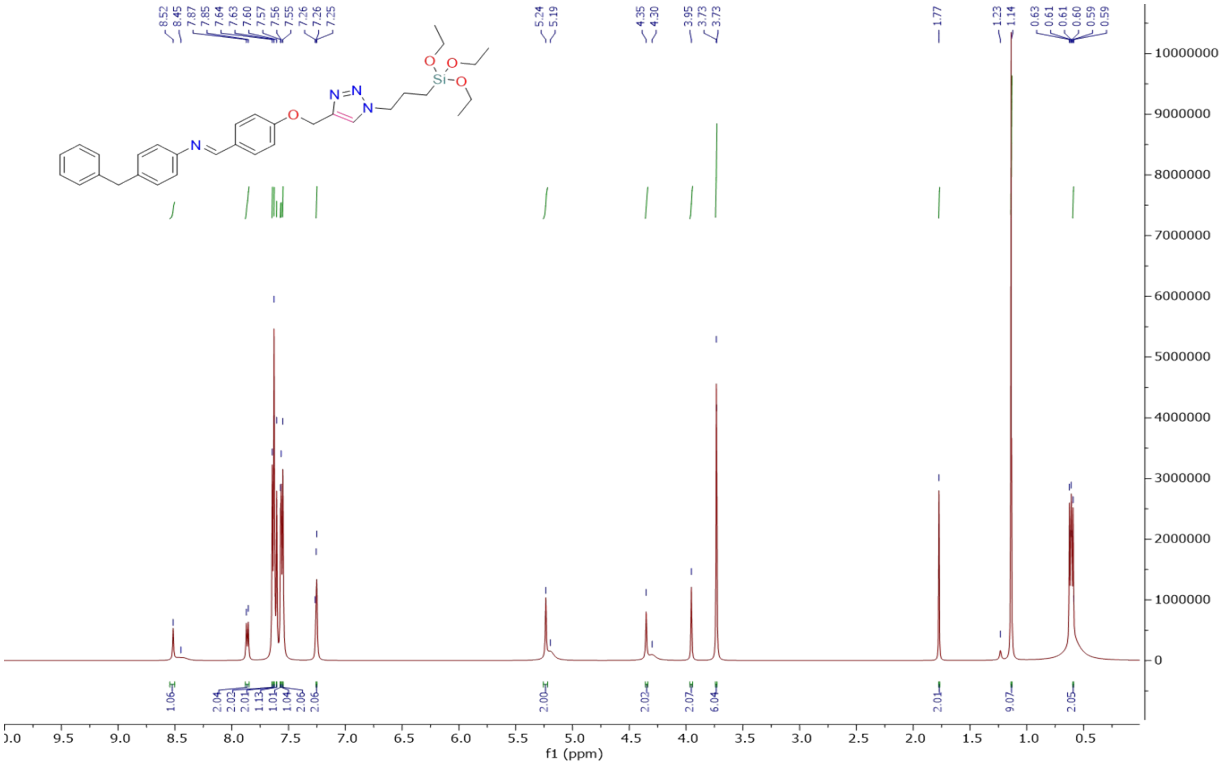

Fig.S5. ^{1}H NMR Spectra of compound 5

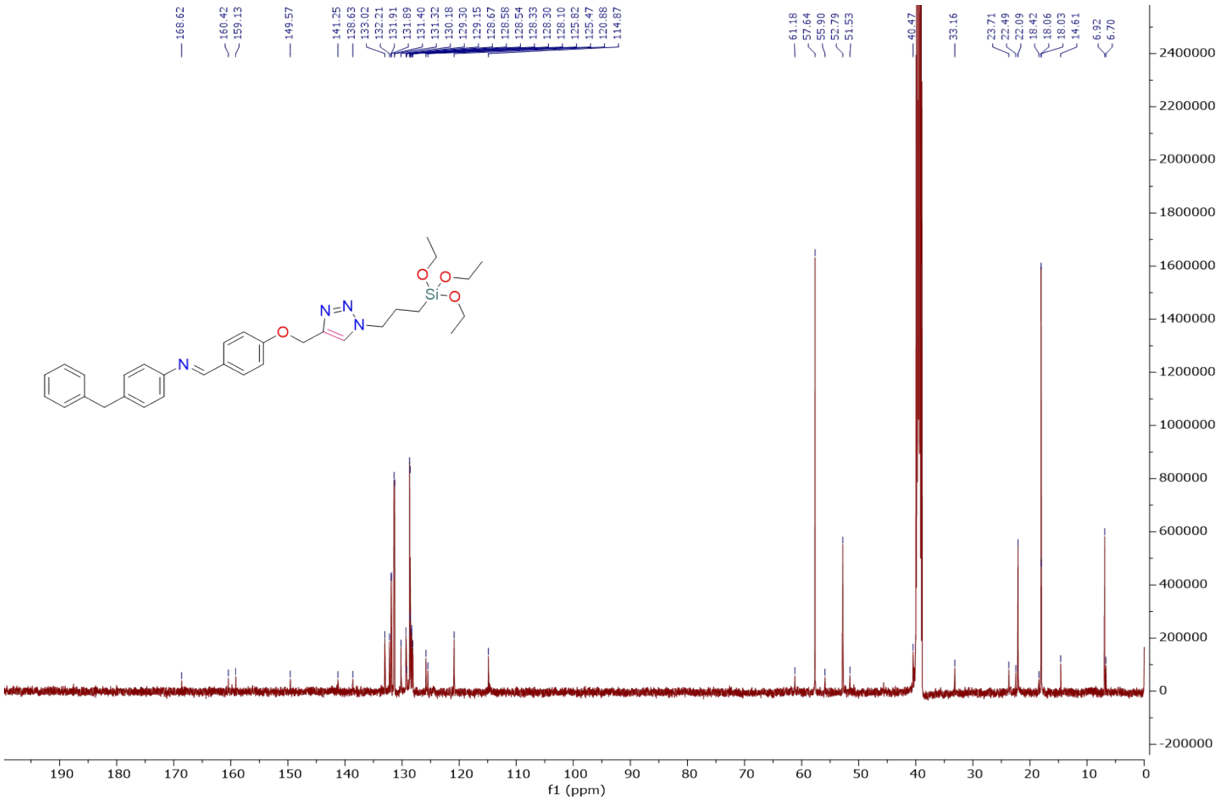

Fig.S6. ^{13}C NMR Spectra of compound 5

Fig. S7. Mass Spectra of compound 5

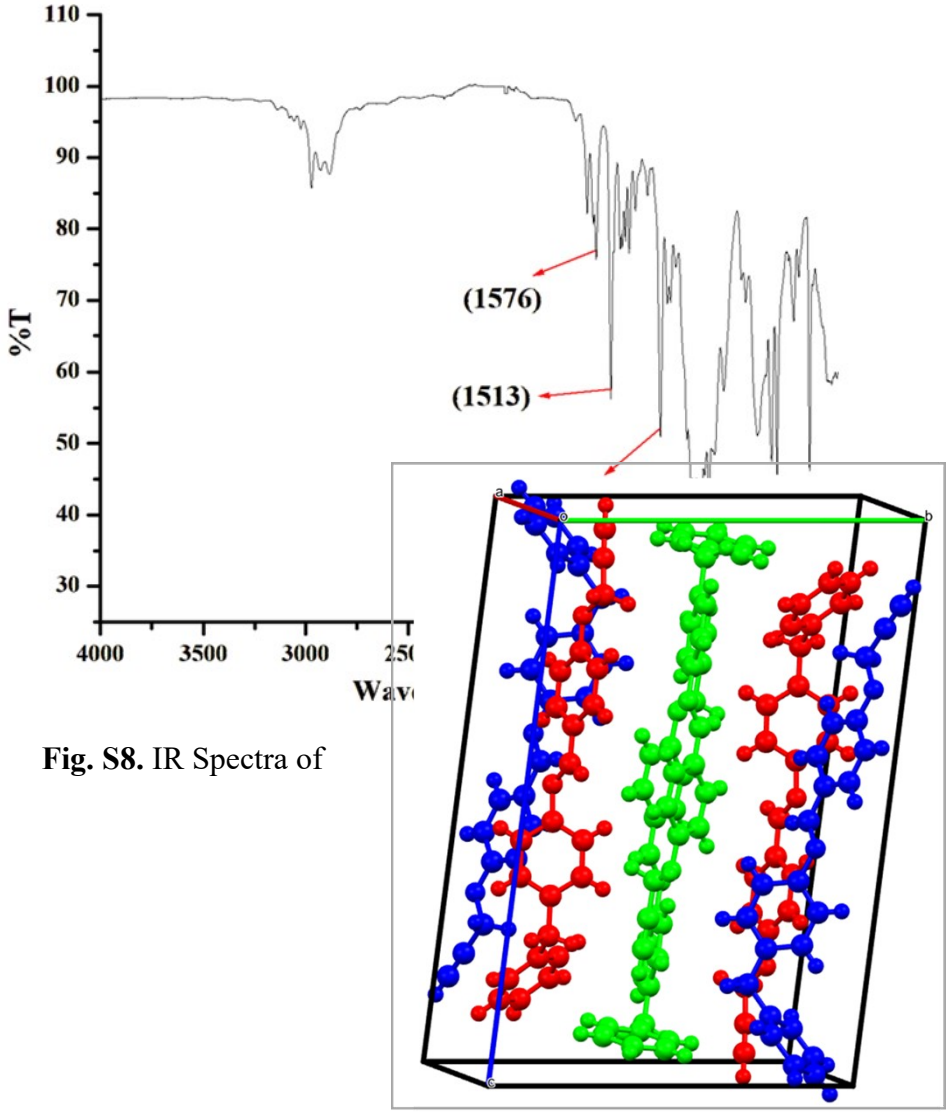

Fig. S8. IR Spectra of compound 5

Fig. S9. Crystal Structure

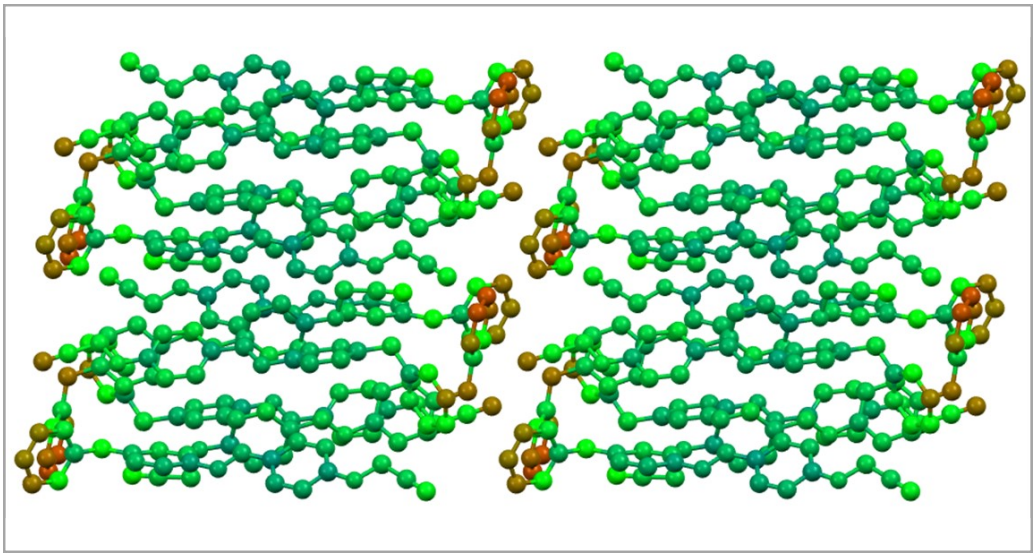

Fig. S10. Crystal structure

Table S1 Bond Lengths for Compound 4.

Atom	Atom	Length/ Å	Atom	Atom	Length/Å
O2	C27	1.374(3)	C60	C59	1.389(4)

Table S1 Bond Lengths for Compound 4.

Atom	Atom	Length/ Å	Atom	Atom	Length/Å
O2	C26	1.426(3)	C60	C61	1.376(4)
O3	C50	1.366(3)	C60	C63	1.514(4)
O3	C49	1.418(3)	C39	C34	1.388(4)
O1	C4	1.369(3)	C39	C38	1.383(4)
O1	C3	1.409(3)	C64	C65	1.361(4)
N1	C57	1.410(3)	C64	C63	1.486(4)
N1	C56	1.272(3)	C64	C70	1.383(4)
N3	C10	1.271(3)	C62	C61	1.377(4)
N3	C11	1.416(3)	C11	C12	1.376(4)
N2	C34	1.417(3)	C48	C49	1.450(4)
N2	C33	1.260(3)	C48	C47	1.166(4)
C57	C58	1.384(3)	C32	C31	1.375(4)
C57	C62	1.385(4)	C12	C13	1.376(4)
C27	C28	1.387(4)	C34	C35	1.375(4)
C27	C32	1.368(4)	C8	C9	1.363(4)
C50	C55	1.382(3)	C36	C35	1.367(4)
C50	C51	1.373(4)	C36	C37	1.379(4)
C56	C53	1.456(4)	C25	C26	1.440(4)
C7	C10	1.453(4)	C25	C24	1.153(4)
C7	C8	1.384(4)	C42	C41	1.370(4)
C7	C6	1.380(4)	C42	C43	1.355(5)
C53	C54	1.384(3)	C42	C40	1.510(4)
C53	C52	1.390(4)	C6	C5	1.370(4)
C30	C29	1.378(4)	C19	C20	1.378(4)
C30	C33	1.467(4)	C38	C37	1.374(4)

Table S1 Bond Lengths for Compound 4.

Atom	Atom	Length/ Å	Atom	Atom	Length/Å
C30	C31	1.381(4)	C37	C40	1.514(4)
C4	C9	1.374(4)	C65	C67	1.351(4)
C4	C5	1.370(4)	C41	C46	1.359(5)
C16	C11	1.379(4)	C21	C20	1.362(4)
C16	C15	1.374(4)	C21	C22	1.351(5)
C18	C19	1.375(4)	C2	C3	1.446(5)
C18	C17	1.504(4)	C2	C1	1.155(4)
C18	C23	1.378(4)	C23	C22	1.384(4)
C55	C54	1.368(3)	C43	C44	1.385(6)
C58	C59	1.376(3)	C70	C69	1.429(5)
C51	C52	1.381(3)	C68	C69	1.354(5)
C14	C13	1.378(4)	C68	C67	1.329(5)
C14	C15	1.385(4)	C46	C45	1.346(6)
C14	C17	1.508(4)	C44	C45	1.371(6)
C28	C29	1.374(4)			

Table S2 Bond Angles for Compound 4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C27	O2	C26	118.2(2)	C12	C11	C16	118.1(3)

Table S2 Bond Angles for Compound 4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C50	O3	C49	119.0(2)	C28	C29	C30	121.7(3)
C4	O1	C3	117.3(2)	C47	C48	C49	179.3(3)
C56	N1	C57	120.5(2)	C51	C52	C53	122.1(3)
C10	N3	C11	119.0(2)	C27	C32	C31	119.6(3)
C33	N2	C34	119.2(3)	C58	C59	C60	122.1(3)
C58	C57	N1	118.1(3)	C11	C12	C13	121.0(3)
C58	C57	C62	117.6(3)	C39	C34	N2	123.0(3)
C62	C57	N1	124.0(3)	C35	C34	N2	118.4(3)
O2	C27	C28	124.7(3)	C35	C34	C39	118.5(3)
C32	C27	O2	114.9(3)	N2	C33	C30	123.4(3)
C32	C27	C28	120.4(3)	C32	C31	C30	121.5(3)
O3	C50	C55	114.8(3)	C9	C8	C7	121.3(3)
O3	C50	C51	125.1(3)	C12	C13	C14	121.5(3)
C51	C50	C55	120.1(3)	O3	C49	C48	107.9(2)
N1	C56	C53	122.2(3)	C35	C36	C37	122.0(3)
C8	C7	C10	122.5(3)	C8	C9	C4	120.6(3)
C6	C7	C10	120.8(3)	C24	C25	C26	177.9(4)
C6	C7	C8	116.7(3)	O2	C26	C25	107.9(3)
C54	C53	C56	121.1(3)	C36	C35	C34	120.5(3)
C54	C53	C52	116.9(3)	C41	C42	C40	121.0(4)
C52	C53	C56	122.0(3)	C43	C42	C41	118.5(4)
C29	C30	C33	121.0(3)	C43	C42	C40	120.4(4)

Table S2 Bond Angles for Compound 4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C29	C30	C31	117.9(3)	C16	C15	C14	121.8(3)
C31	C30	C33	121.0(3)	C5	C6	C7	122.8(3)
O1	C4	C9	116.1(3)	C18	C19	C20	121.2(3)
O1	C4	C5	124.4(3)	C37	C38	C39	121.5(3)
C5	C4	C9	119.6(3)	C60	C61	C62	122.2(3)
N3	C10	C7	124.2(3)	C36	C37	C40	118.8(3)
C15	C16	C11	120.6(3)	C38	C37	C36	117.4(3)
C19	C18	C17	121.2(3)	C38	C37	C40	123.7(3)
C19	C18	C23	117.6(3)	C6	C5	C4	119.0(3)
C23	C18	C17	121.2(3)	C18	C17	C14	115.0(2)
C54	C55	C50	119.8(3)	C67	C65	C64	123.0(4)
C59	C58	C57	120.7(3)	C46	C41	C42	121.0(4)
C50	C51	C52	119.2(3)	C22	C21	C20	119.1(3)
C13	C14	C15	116.9(3)	C1	C2	C3	177.6(4)
C13	C14	C17	122.0(3)	C21	C20	C19	120.5(3)
C15	C14	C17	121.1(3)	C18	C23	C22	120.6(3)
C55	C54	C53	121.9(3)	O1	C3	C2	109.0(3)
C29	C28	C27	118.9(3)	C42	C43	C44	121.2(4)
C59	C60	C63	123.9(3)	C64	C63	C60	115.7(3)
C61	C60	C59	116.4(3)	C64	C70	C69	119.9(4)
C61	C60	C63	119.7(3)	C67	C68	C69	122.8(4)
C38	C39	C34	120.0(3)	C68	C69	C70	117.5(4)

Table S2 Bond Angles for Compound 4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C65	C64	C63	119.8(3)	C68	C67	C65	119.3(4)
C65	C64	C70	117.5(3)	C21	C22	C23	121.1(4)
C70	C64	C63	122.7(4)	C45	C46	C41	120.0(5)
C61	C62	C57	120.9(3)	C42	C40	C37	116.7(3)
C16	C11	N3	118.4(3)	C45	C44	C43	118.4(5)
C12	C11	N3	123.4(3)	C46	C45	C44	120.7(6)

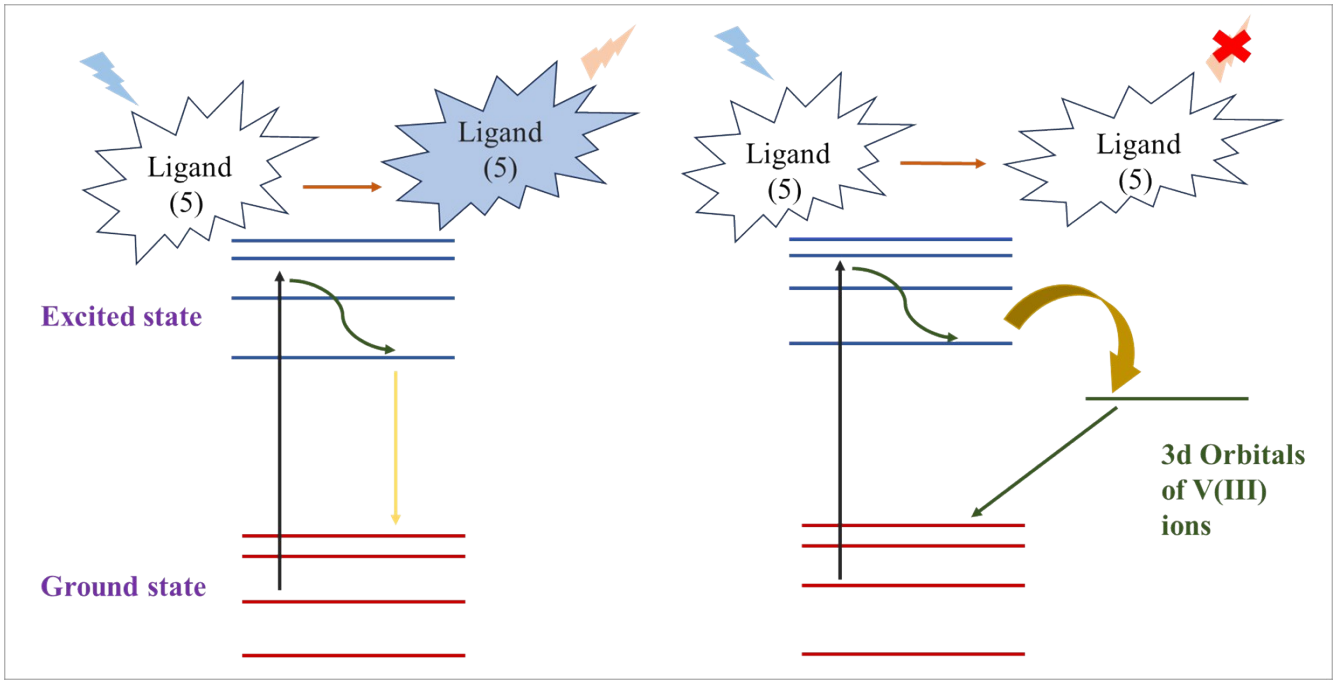

Fig.S11. Fluorescence quenching mechanism for ligand (5).

Table S3. % cell viability under control and in presence of (5)

Biological Replicate 1

Name	Control	(5)
1	0.91	0.98
2	1.40	0.82
3	1.38	0.88
Avg		

Name	Control	(5)
1	0.18	0.82
2	1.44	0.87
3	1.28	0.91
Avg		0.87

After removing outliers

Biological Replicate 2

Name	Control	(5)
1		
2	1.40	0.82
3	1.38	0.88
Avg	1.39	0.85
% Viability	100	61.20

Name	Control	(5)
1		0.82
2	1.44	0.87
3	1.28	0.91
Avg	1.36	0.87
% Viability	100	63.61

Conclusion

Name	Control	Ligand (5)	Ligand (4)
1	100	61.20	22.71
2	100	63.61	21.40
Avg.	100	62.40	22.06
Standard Deviation	0	1.70	0.92

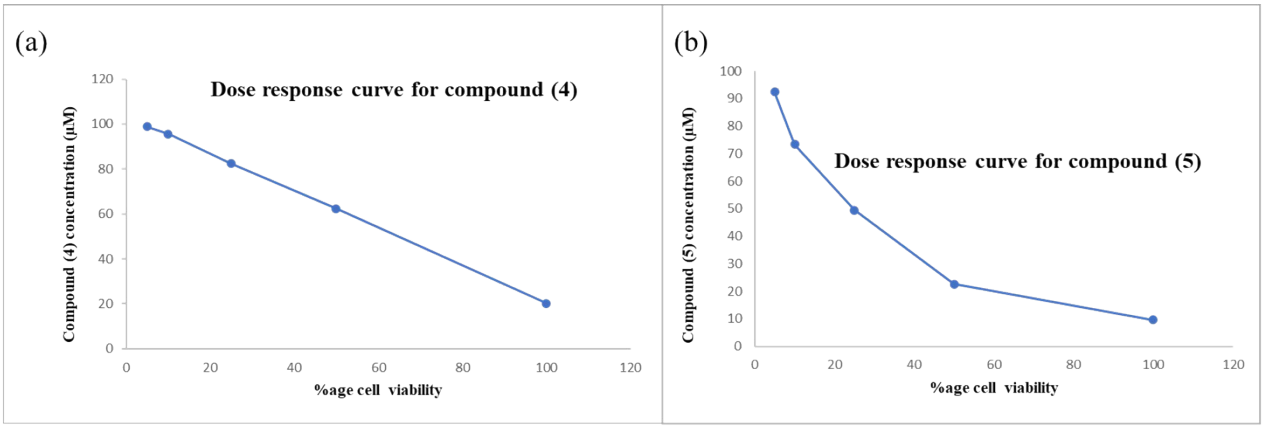

Fig.S12. Dose response curve for compound (4) and (5).

Table S4. Molecular Docking Table

Hydrophobic Interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	571A	ILE	2.94	2923	73
2	595A	LEU	4.00	2940	330
3	603A	VAL	3.33	2934	391
4	603A	VAL	2.95	2938	390
5	621A	ALA	3.06	2938	541
6	643A	VAL	3.52	2923	754
7	644A	LEU	3.63	2909	763
8	654A	VAL	2.97	2909	869
9	654A	VAL	3.29	2937	866
10	789A	ILE	3.26	2929	1470
11	791A	ARG	3.87	2918	1490
12	799A	LEU	3.60	2941	1575
13	799A	LEU	3.03	2943	1576

14	810A	ASP	3.33	2905	1682
15	811A	PHE	3.70	2943	1697

Hydrogen Bonds

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	623A	LYS	3.30	3.95	123.42			559 [N3+]	2931 [N2]
2	789A	ILE	2.59	3.43	139.86			1462 [Nam]	2927 [O3]
3	791A	ARG	2.99	3.99	167.01			1492 [Ng+]	2927 [O3]
4	810A	ASP	2.54	3.50	156.59			1677 [Nam]	2931 [N2]

π-Stacking

Index	Residue	AA	Distance	Angle	Offset	Stacking Type	Ligand Atoms
1	790A	HIS	4.80	65.09	1.13	T	2912, 2913, 2914, 2915, 2916

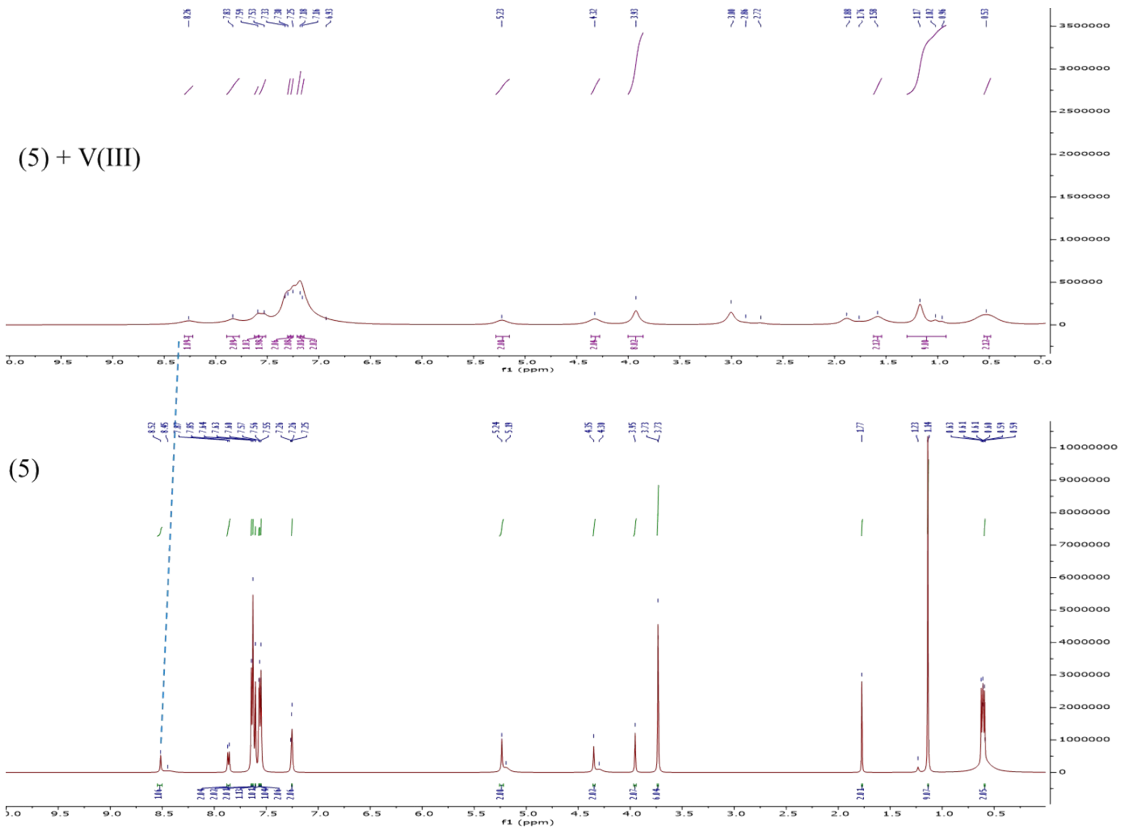

Fig. S13. Comparison of ^{1}H NMR Spectra of (5) and (5) + V(III)

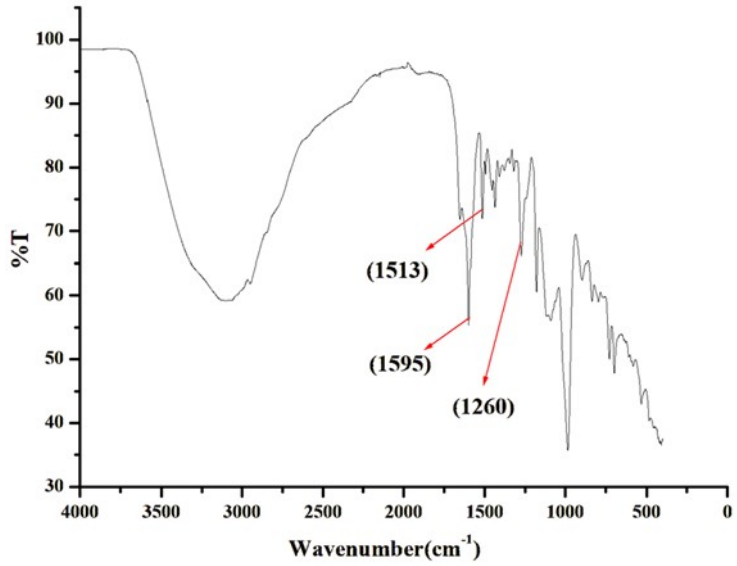

Fig.S14. IR Spectra of complex

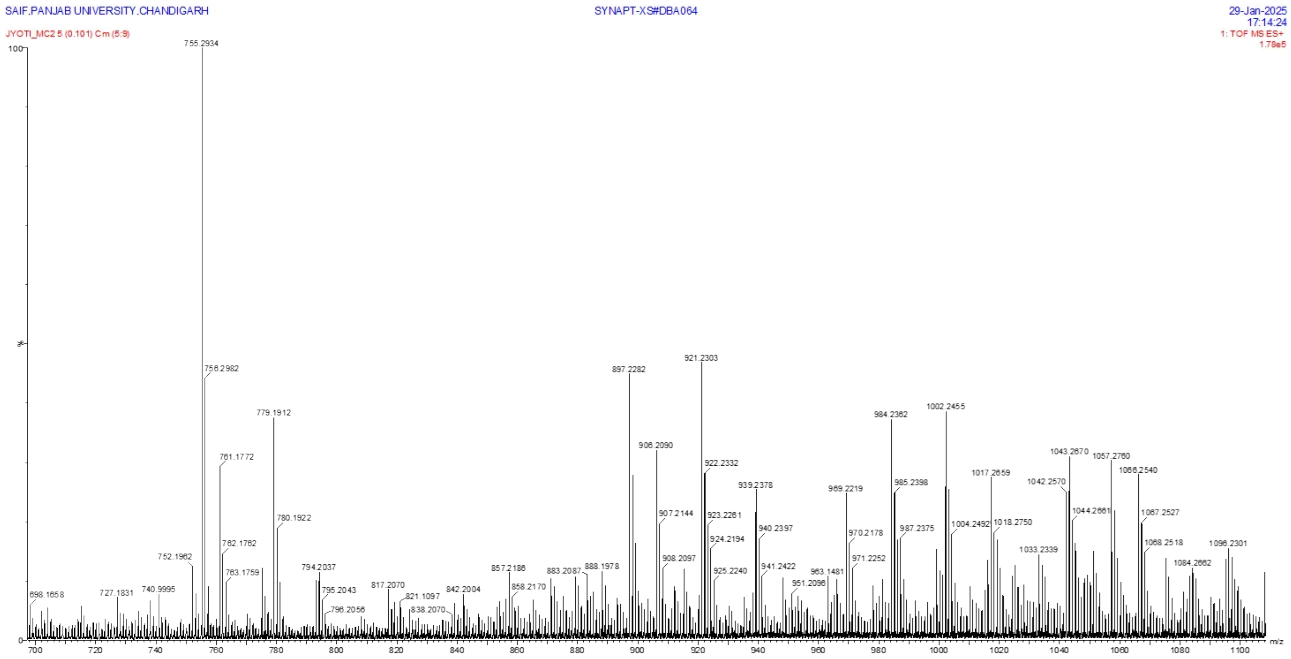

Fig. S15. Mass Spectra of Complex