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Supporting information

Zinc(II) Complexes with Uncommon Aminal and Hemiaminal Ether Derivative: Synthesis, Structure, Phosphatase Activity and Theoretical Rationalization of Ligand and Complex Formation

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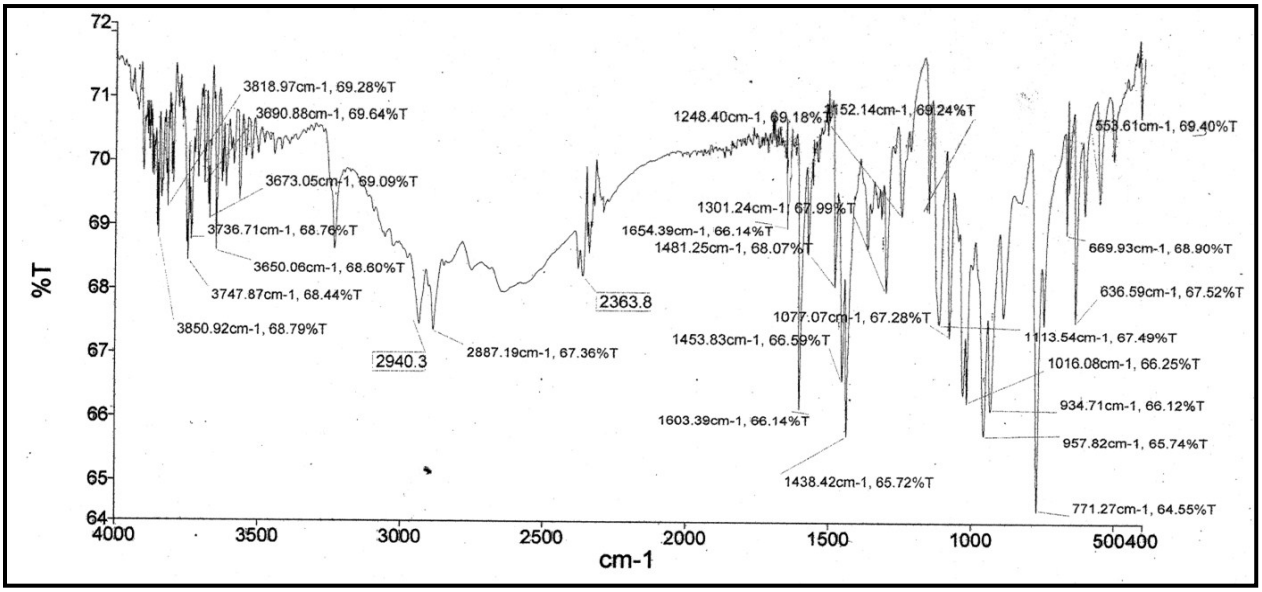

Fig. S1 IR Spectrum of Complex **1.**

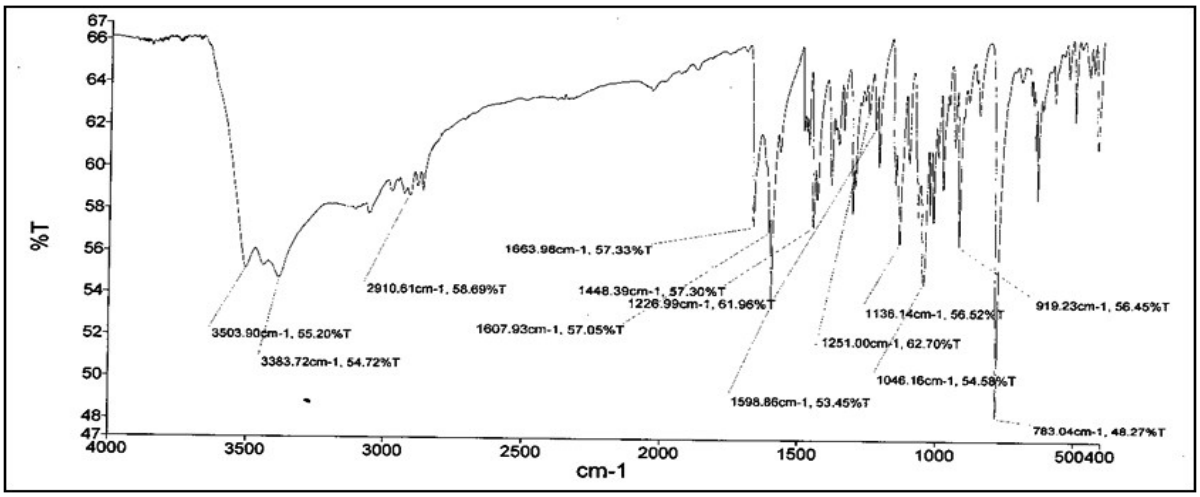

Fig. S2 IR Spectrum of Complex **2.**

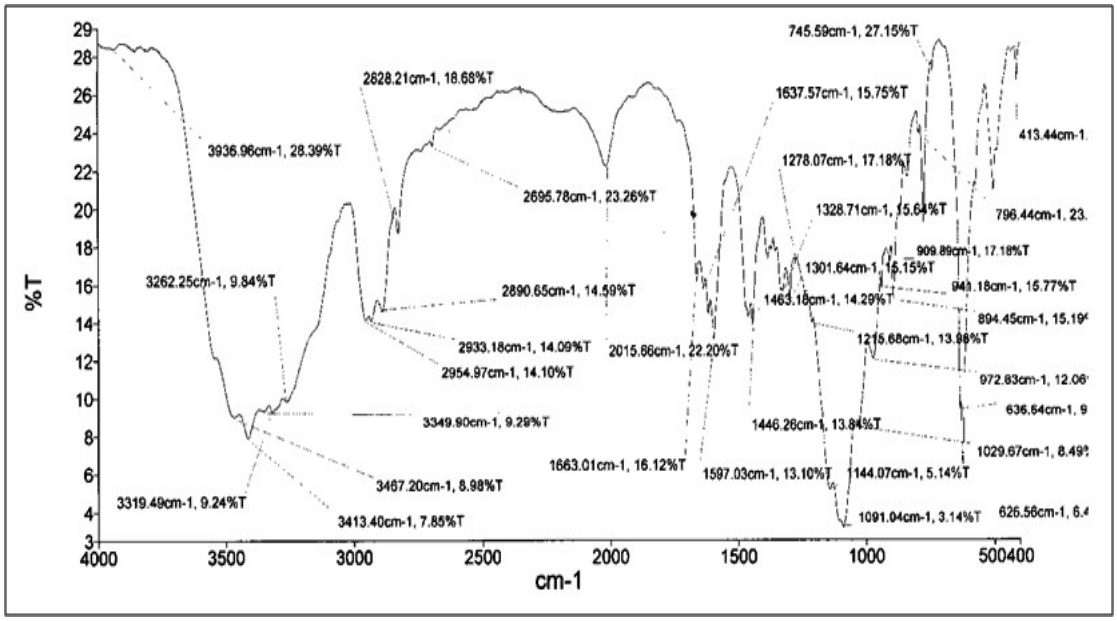

Fig. S3 IR Spectrum of Complex **3.**

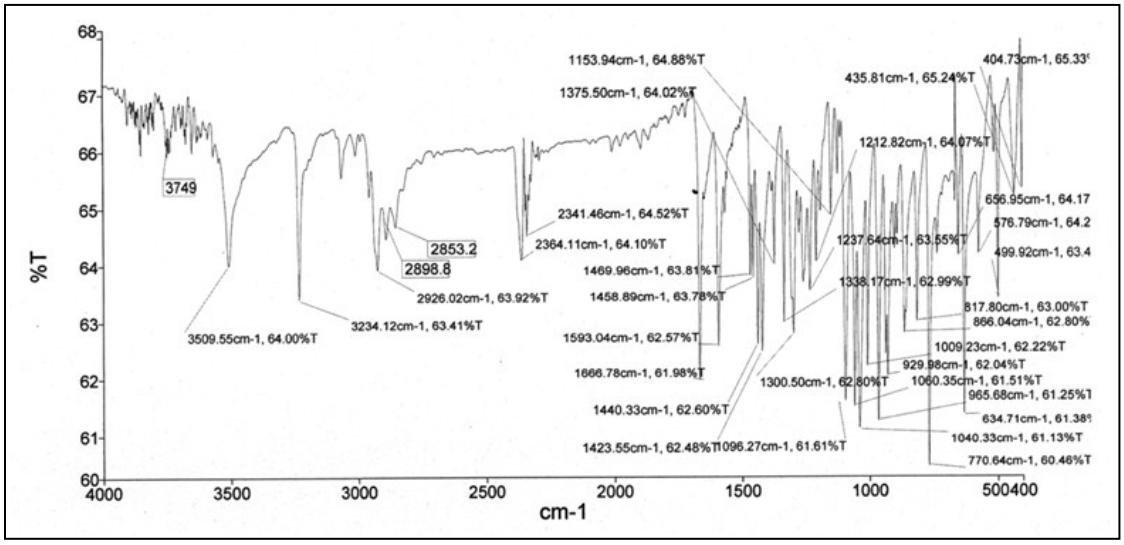

Fig. S4 IR Spectrum of Complex **4.**

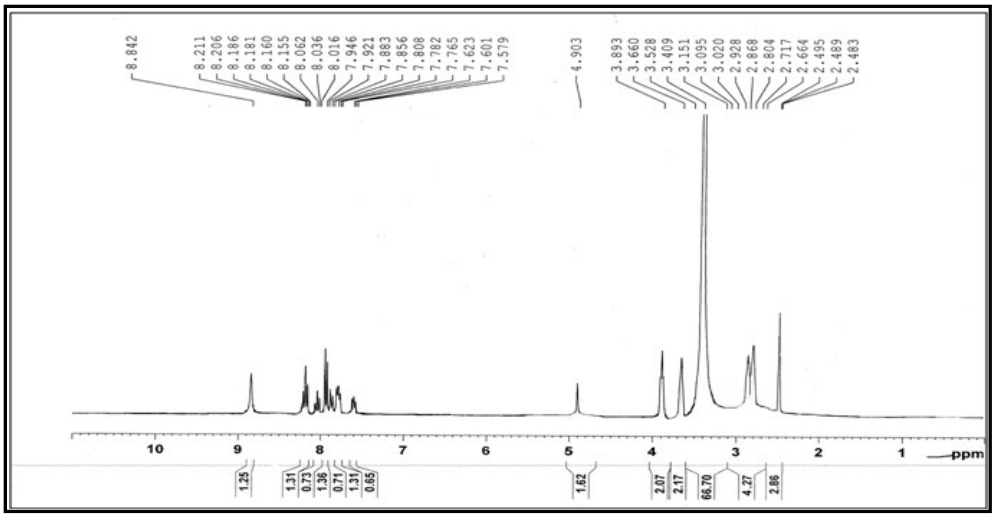

Fig. S5 ^{1}H NMR Spectrum of ligand L**.**

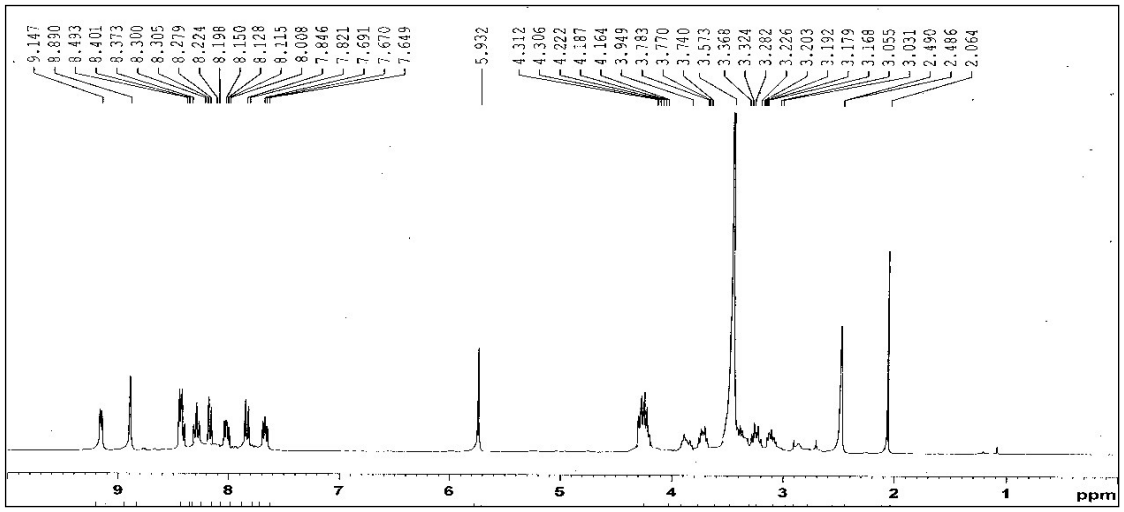

Fig. S6 ^{1}H NMR Spectrum of Complex **2.**

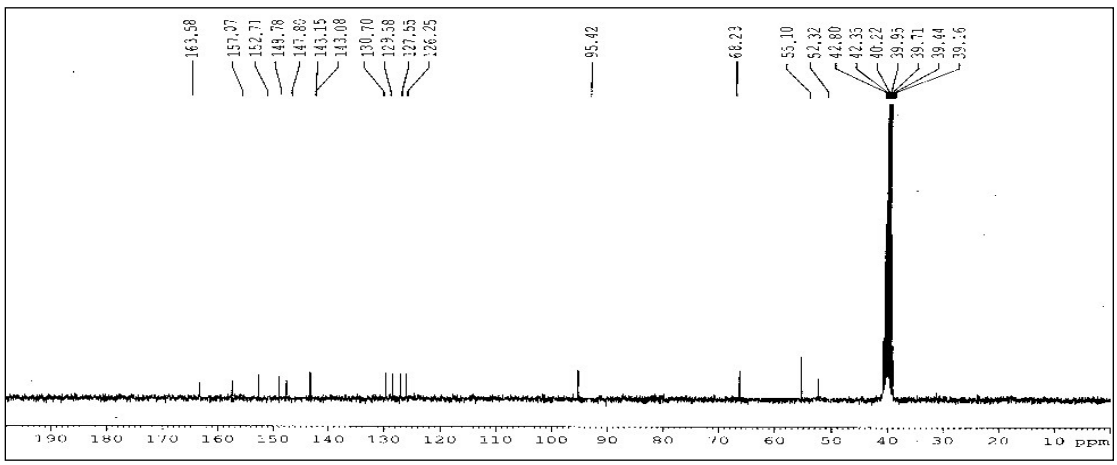

Fig. S7 ^{13}C -NMR Spectrum of Complex **2.**

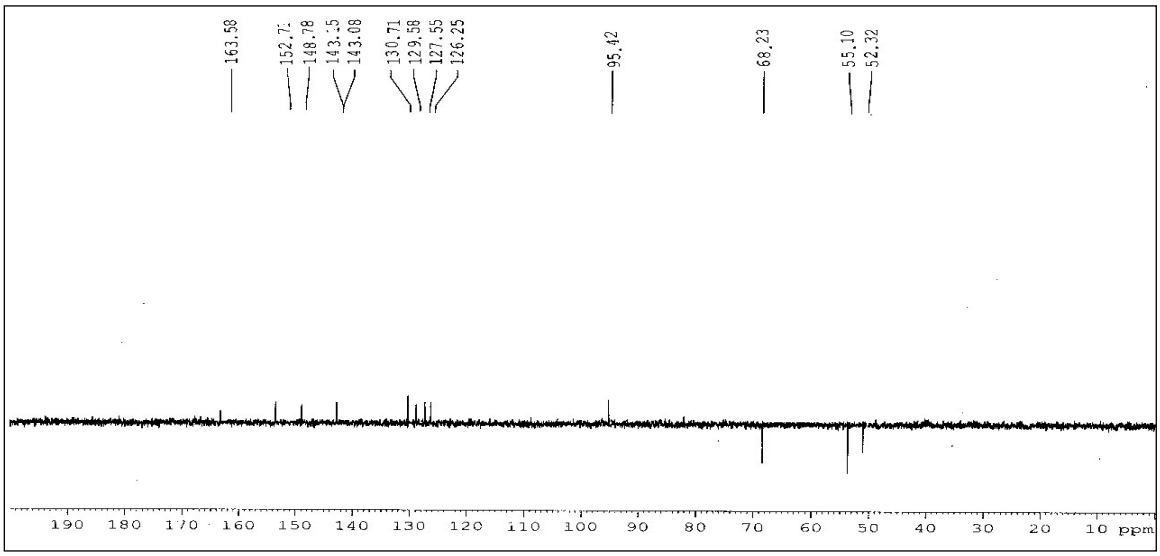

Fig. S8 DEPT-135 Spectrum of Complex **2.**

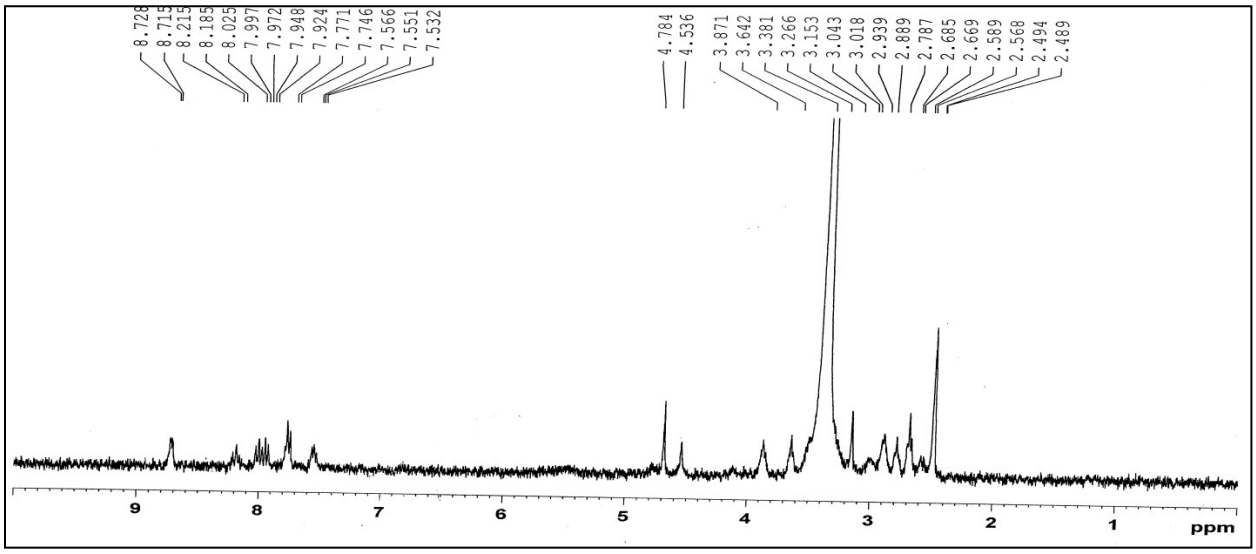

Fig. S9 ^{1}H- NMR Spectrum of Complex **4.**

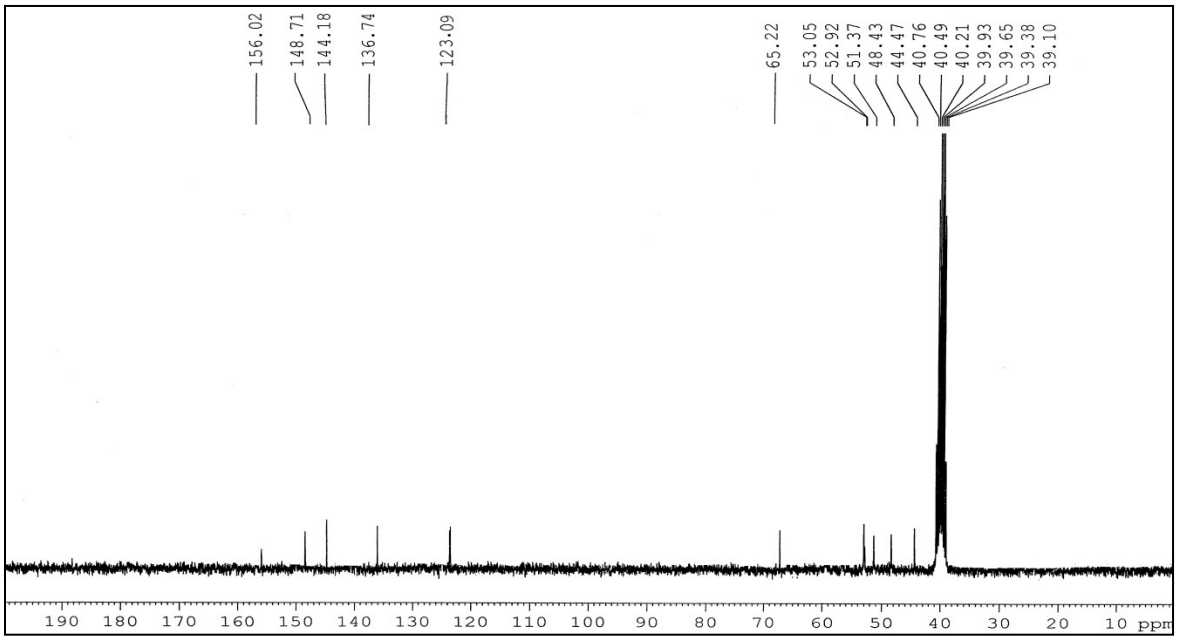

Fig.S10 ^{13}C- NMR Spectrum of Complex **4.**

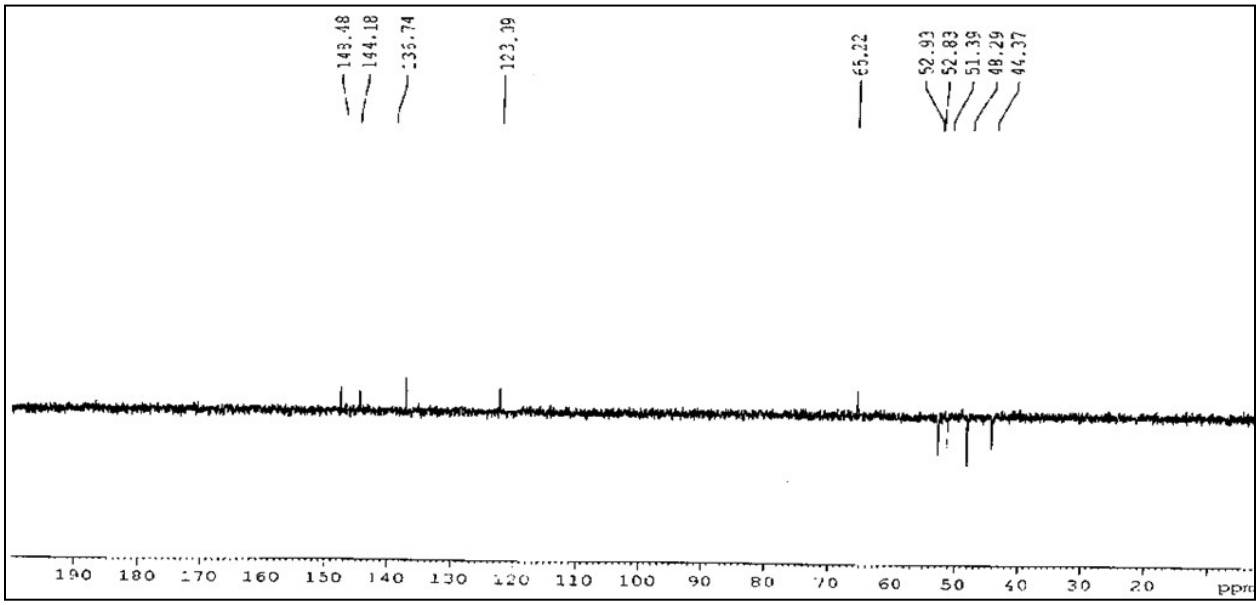

Fig. S11 DEPT-135 Spectrum of Complex **4.**

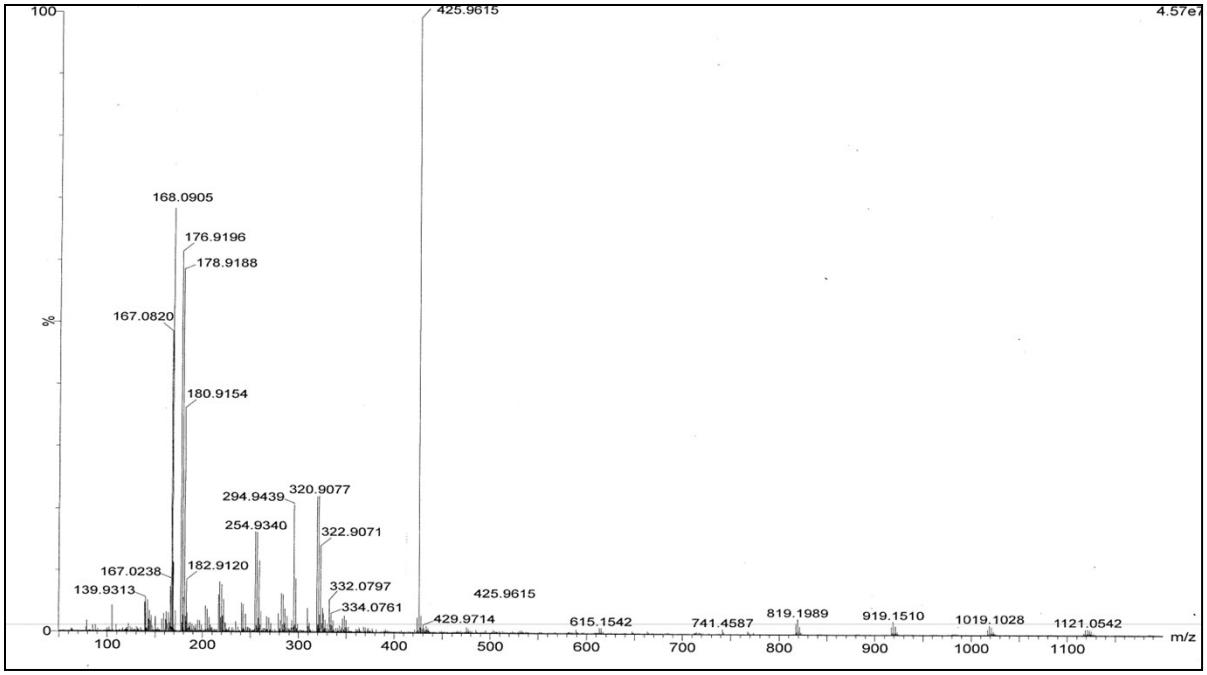

Fig. S12 Mass Spectrum of Complex **1.**

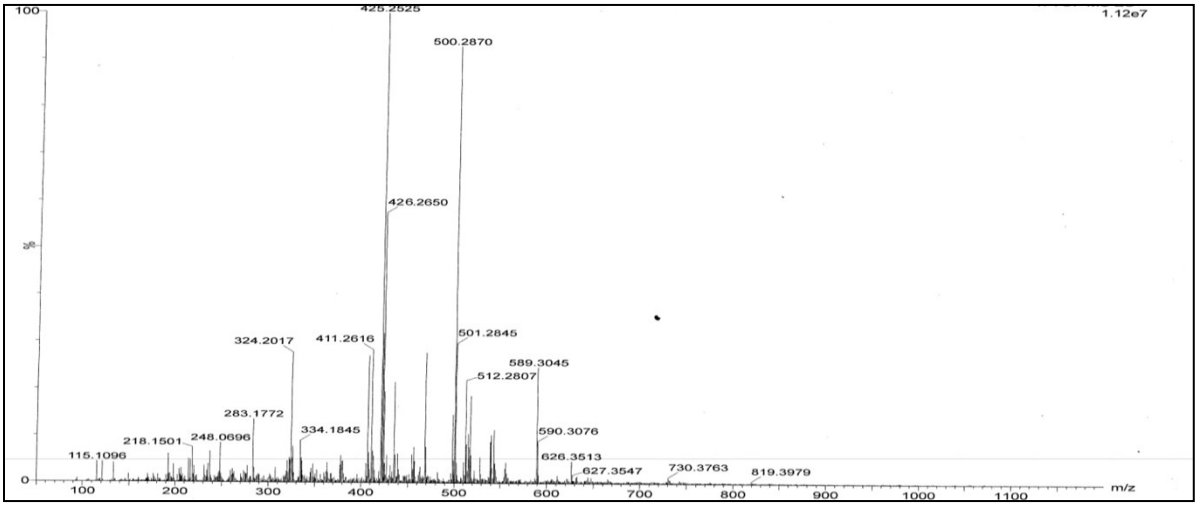

Fig.S13 Mass Spectrum of Complex **2.**

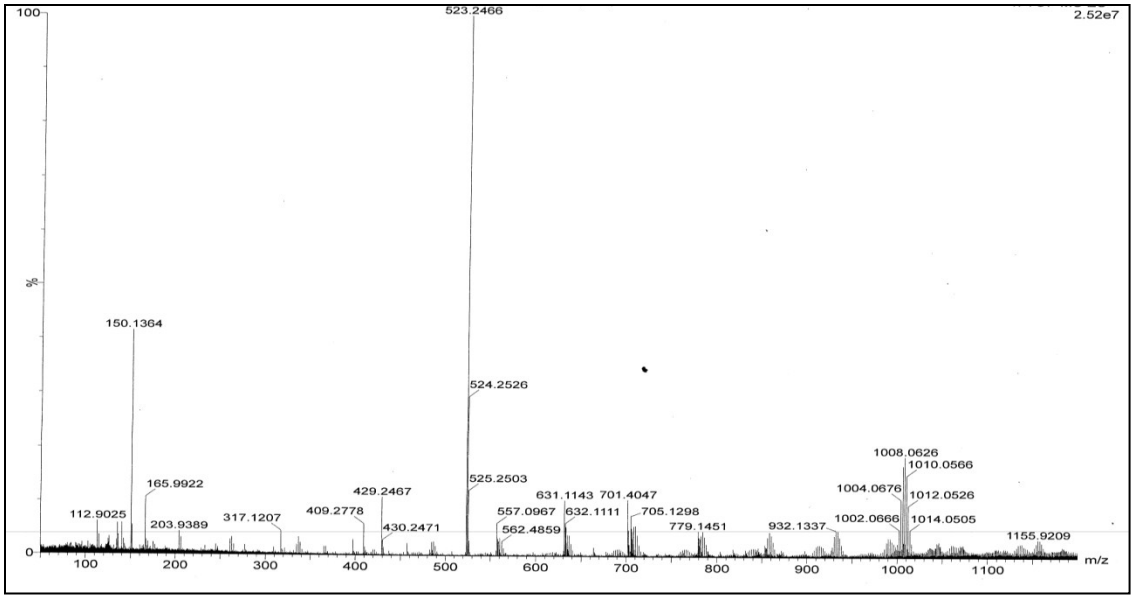

Fig. S14 Mass Spectrum of Complex **3.**

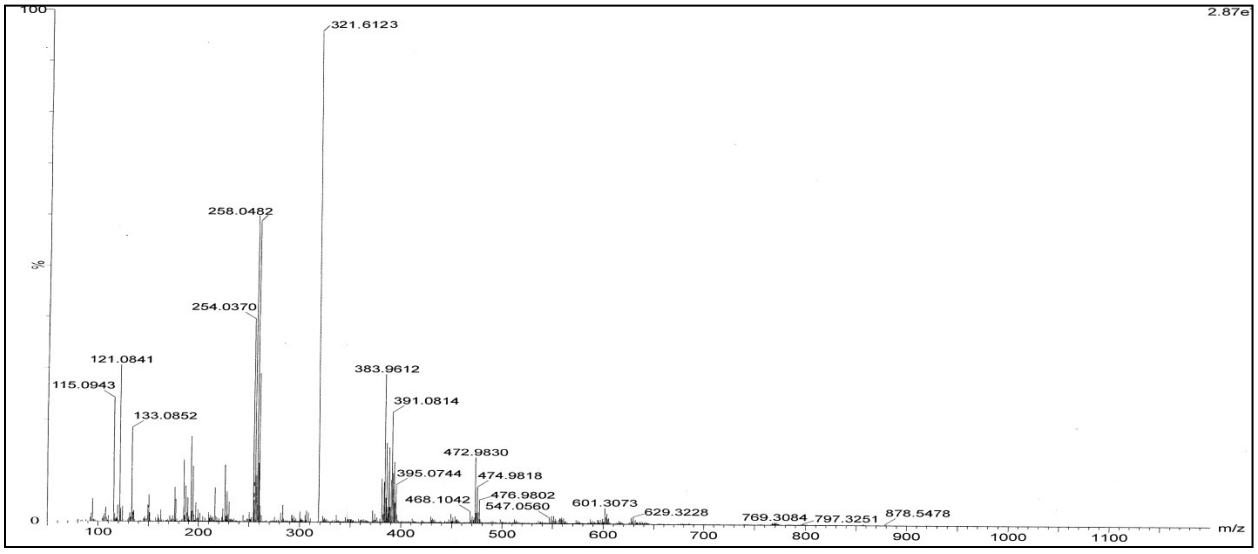

Fig. S15 Mass Spectra of Complex **4**.

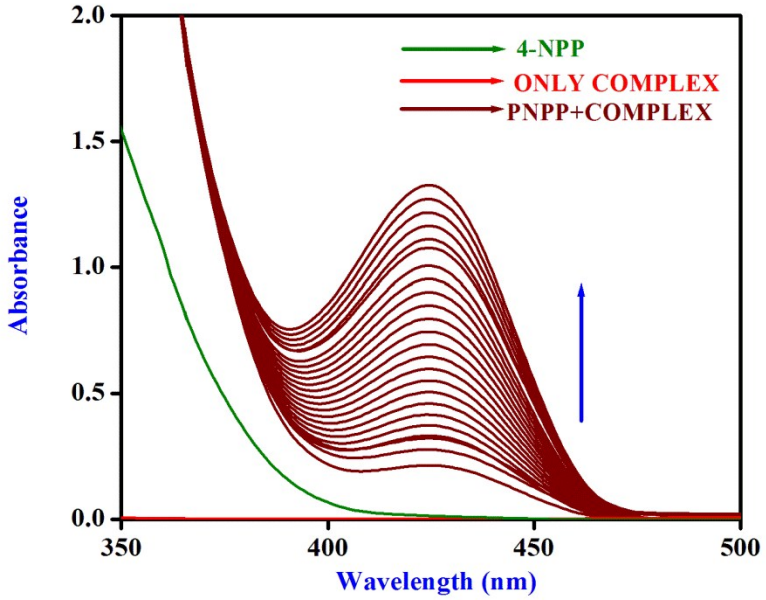

Fig. S16 Wavelength scan for the hydrolysis of 4-NPP in the absence and presence of complex 2(substrate: catalyst =20:1) in 97.5% DMF recorded at 25 °C at an interval of 5 min for 2 h.

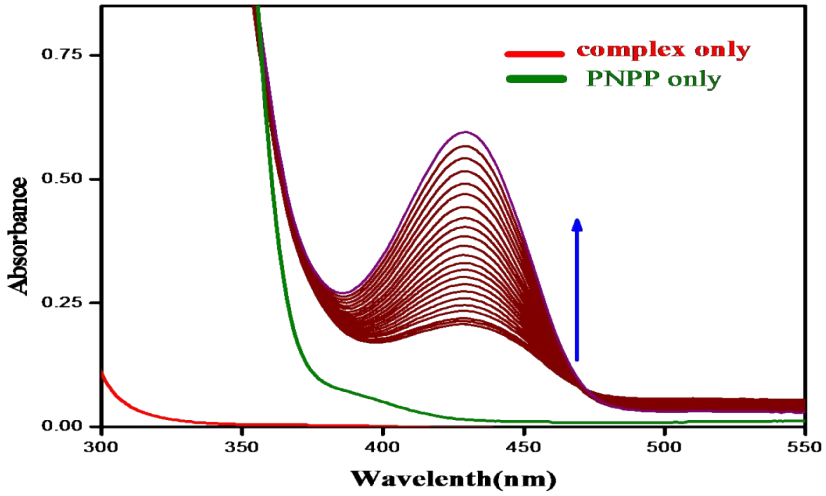

Fig. S17 Wavelength scan for the hydrolysis of 4-NPP in the absence and presence of complex 3(substrate: catalyst =20:1) in 97.5% DMF recorded at 25 °C at an interval of 5 min for 2 h.

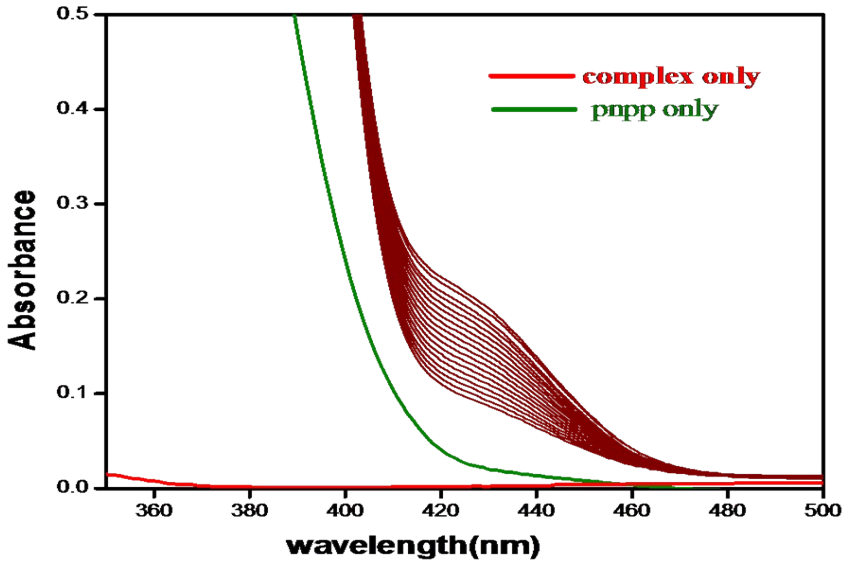

Fig. S 18 Wavelength scan for the hydrolysis of 4-NPP in the absence and presence of complex 4(substrate: catalyst =20:1) in 97.5% DMF recorded at 25 °C at an interval of 5 min for 2 h.

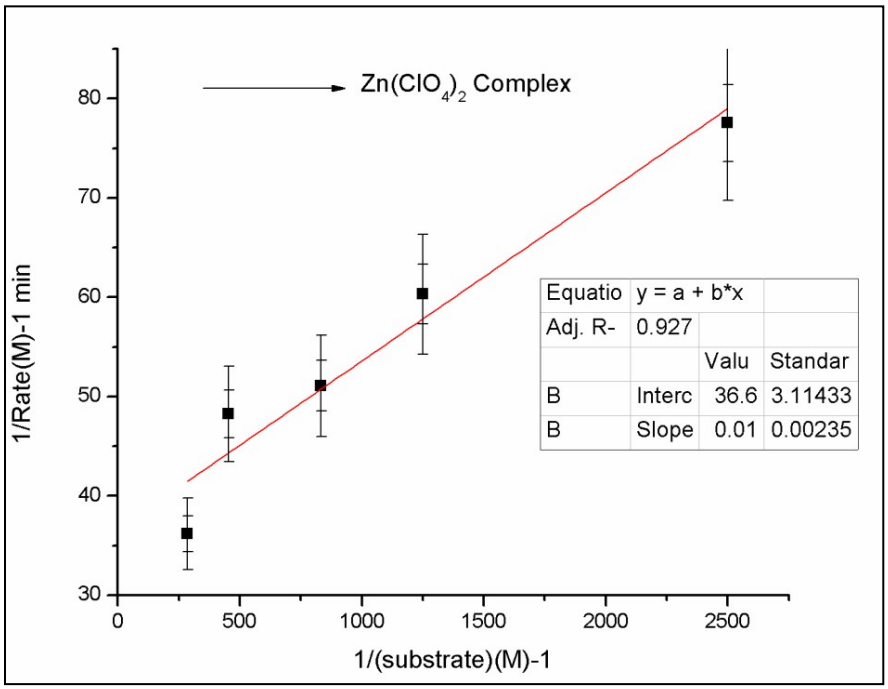

Fig. S19 Lineweaver−Burk plot of Complex **1.**

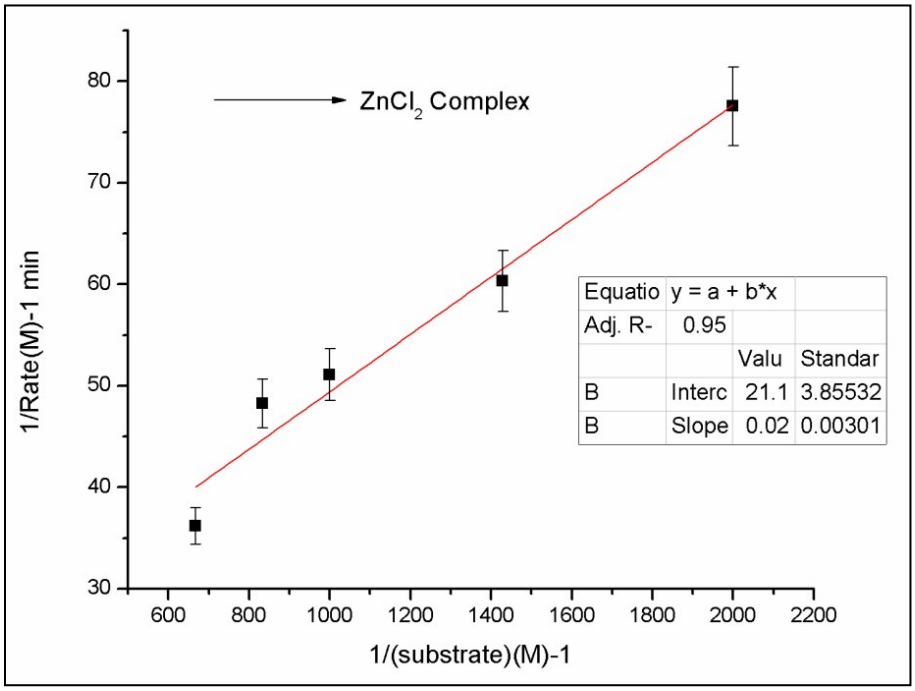

Fig. S20 Lineweaver−Burk plot of Complex **2.**

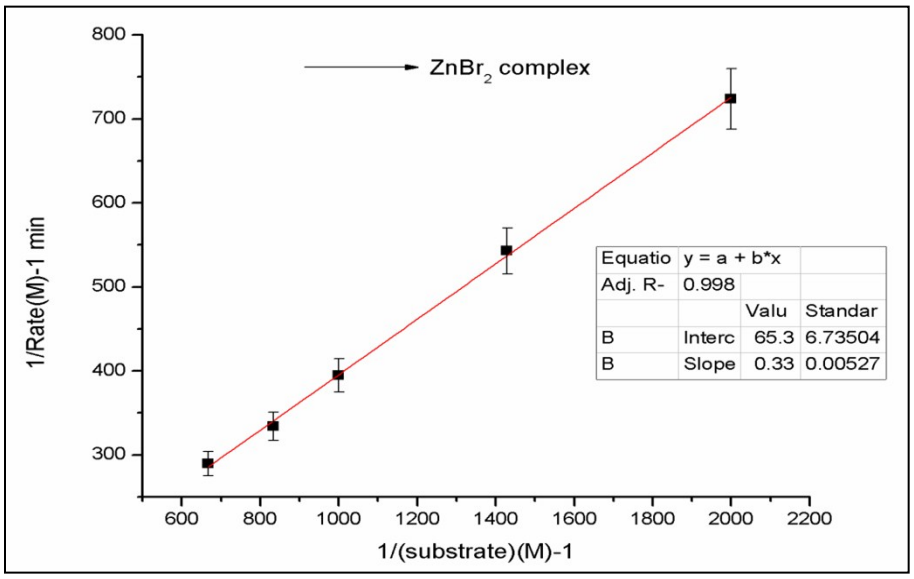

Fig. S21 Lineweaver−Burk plot of Complex **3.**

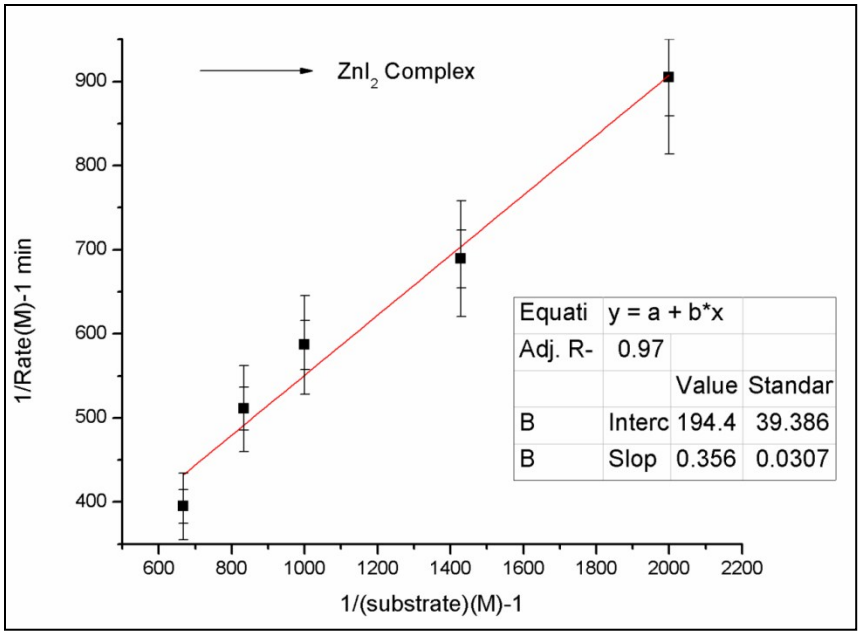

Fig. S22 Lineweaver−Burk plot Complex **4**.

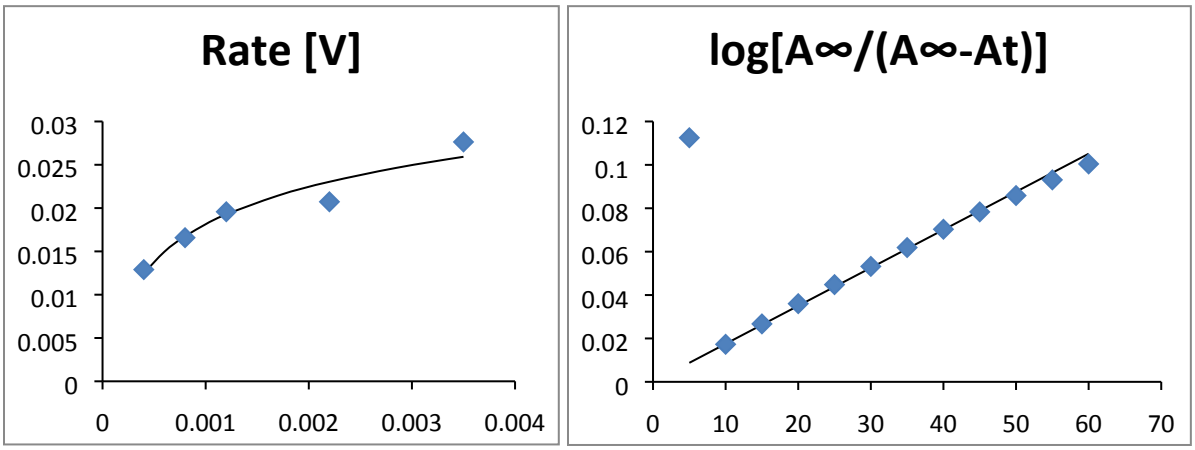

Fig. S23 Plot of Enzymatic Kinetics for Complex **1.**

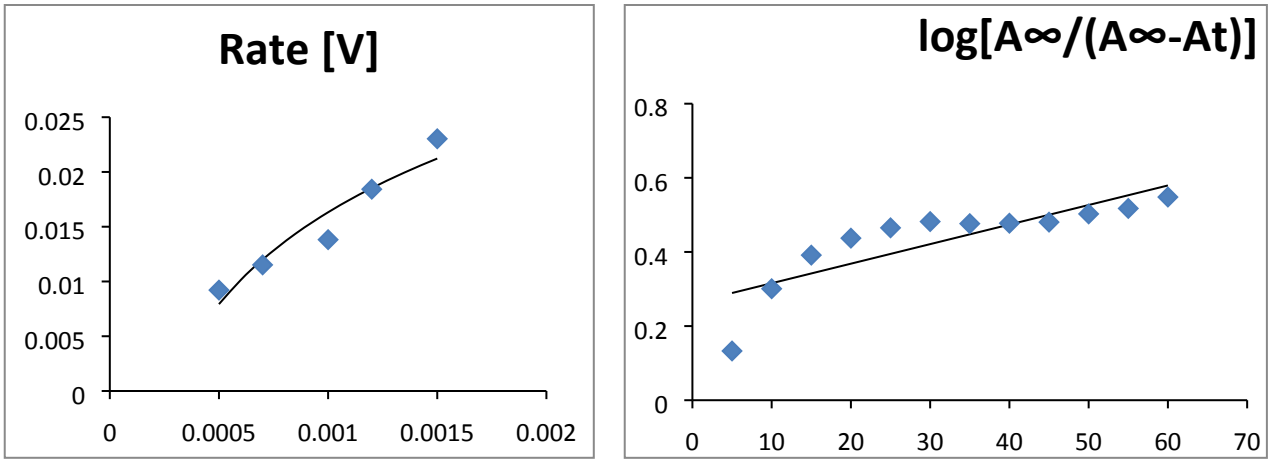

Fig.S24 Plot of Enzymatic Kinetics for Complex **2**

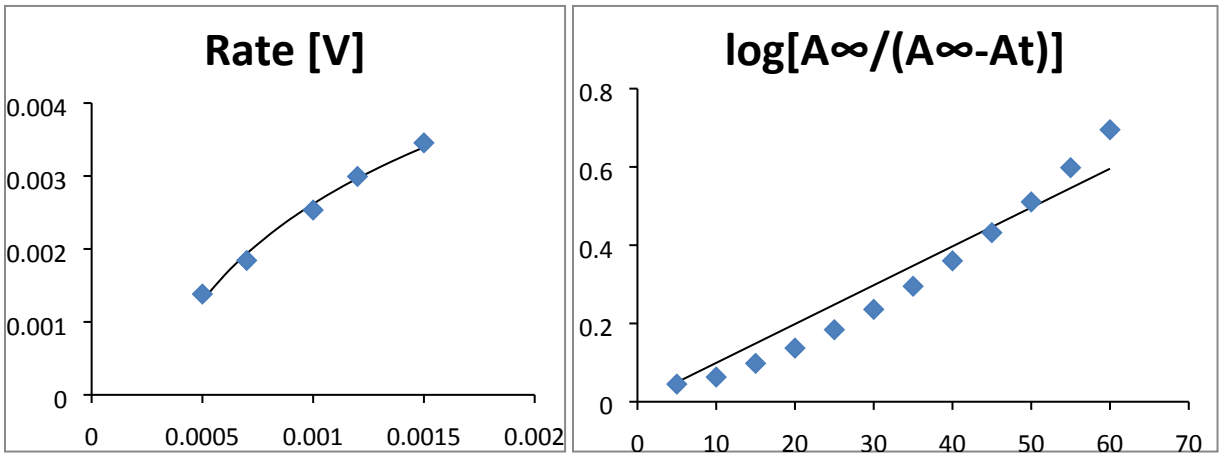

Fig. S25 Plot of Enzymatic Kinetics for Complex **3**

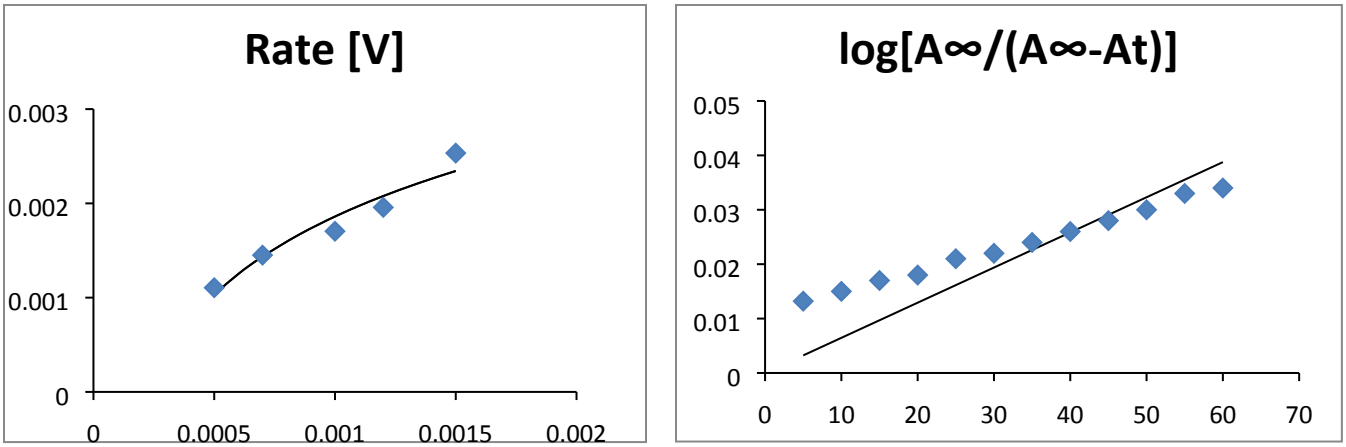

Fig. S26 Plot of Enzymatic Kinetics for Complex **4.**

Table.S27 kinetic data of Time vs log A∞/(A∞-At) of complex 1at PNPP Concentration 0.001.

Time(t)	Abs at 430 nm(At)	Abs at infinity(A∞)	(A∞-At)	A∞/(A∞-At)	log A∞/(A∞-At)
5	0.089	3.478	3.389	1.02626	0.1125
10	0.136		3.342	1.040694	0.0173
15	0.208		3.27	1.063608	0.0267
20	0.277		3.201	1.086535	0.036029
25	0.341		3.137	1.108702	0.04481
30	0.401		3.077	1.13032	0.0532
35	0.462		3.016	1.15318	0.06189
40	0.52		2.958	1.17579	0.07032
45	0.574		2.904	1.197658	0.07833
50	0.624		2.854	1.2186405	0.08586
55	0.671		2.807	1.239045	0.093087
60	0.718		2.76	1.2601449	0.1004204

Table.S28 kinetic data of Time vs log A∞/(A∞-At) of complex 2 at PNPP Concentration 0.001.

Time(t)	Abs at 430nm(At)	Abs at infinity(A∞)	(A∞-At)	A∞/(A∞-At)	Log A∞/(A∞-At)
5	0.928	3.522	2.594	1.35774	0.1328166
10	1.762		1.762	1.9988649	0.30078
15	2.092		1.43	2.462937	0.3914
20	2.235		1.287	2.73659	0.4372097
25	2.315		1.207	2.91797	0.46508
30	2.361		1.161	3.03359	0.481956
35	2.346		1.176	2.994897	0.476381
40	2.349		1.173	3.002557	0.47749126
45	2.357		1.165	3.023175	0.48046
50	2.415		1.107	3.1815	0.502631
55	2.452		1.07	3.2915	0.5173938
60	2.525		0.997	3.5325	0.548082

Table.S29 kinetic data of Time vs log A∞/(A∞-At) of complex 3 at PNPP Concentration 0.001.

Time(min)	Abs at 430nm(At)	Abs at infinity (A∞)	(A∞-At)	A∞/((A∞-at)	log A∞/(A∞-At)
5	0.345	3.533	3.188	1.108218319	0.045
10	0.482		3.051	1.15798099	0.063
15	0.72		2.813	1.255954497	0.098
20	0.962		2.571	1.374173473	0.137
25	1.225		2.308	1.530762565	0.184
30	1.482		2.051	1.722574354	0.236
35	1.744		1.789	1.974846283	0.295
40	1.988		1.545	2.286731392	0.36
45	2.226		1.307	2.703136955	0.432
50	2.443		1.09	3.241284404	0.5105
55	2.642		0.891	3.965207632	0.598
60	2.82		0.713	4.955119215	0.695

Table.S30 kinetic data of Time vs log A∞/(A∞-At) of complex 4 at PNPP Concentration 0.001.

Time(Min)	Abs at 430nm(At)	Abs at infinity(A∞)	(A∞-At)	A∞/(A∞-At)	log A∞/(A∞-At)
5	0.044	1.426	1.382	1.03183792	0.0132
10	0.049		1.377	1.0355846	0.015
15	0.055		1.371	1.0401167	0.017
20	0.06		1.366	1.04392387	0.018
25	0.066		1.36	1.04852941	0.021
30	0.071		1.355	1.05239852	0.022
35	0.077		1.349	1.05707932	0.024
40	0.083		1.343	1.06180194	0.026
45	0.089		1.337	1.06656694	0.028
50	0.095		1.331	1.07137491	0.03
55	0.101		1.325	1.07622642	0.033
60	0.107		1.319	1.08112206	0.034

Table S31. Analysis of π-stacking interactions in Compounds 1 and 3

Cg(1)	Cg(2)	Symmetry Cg(2)	Cg-Cg	α	β	γ	Slippage
compound **1**							
Py(N4)	Py(N4)	[2-x,2-y,2-z]	3.7705(18)	0	21.4	21.4	1.377
compound **3**							
Py(N1)	Py(N1)	[2-x,1-y,1-z]	3.824(10)	0	26.9	26.9	1.733
Py(N4)	Py(N4)	[2-x,2-y,1-z]	3.629(11)	0	21.4	21.4	1.324

Cg-Cg = Distance between ring centroids (Å); α = dihedral angle between planes 1 and 2 (°); β = angle Cg(1)-Cg(2) or Cg(1)-Me vector and normal to plane 1 (°); γ = Angle Cg(1)-Cg(2) vector and normal to plane 2 (°);Slippage = Distance between Cg(1) and Perpendicular Projection of Cg(2) on Ring 1 (Å).