

Supporting Information

Lower rim 1,3-di-derivative of calix[4]arene appended salicylidene imine (H₂L): Experimental and computational studies of the selective recognition of H₂L towards Zn²⁺, and sensing phosphate and amino acid by [ZnL]

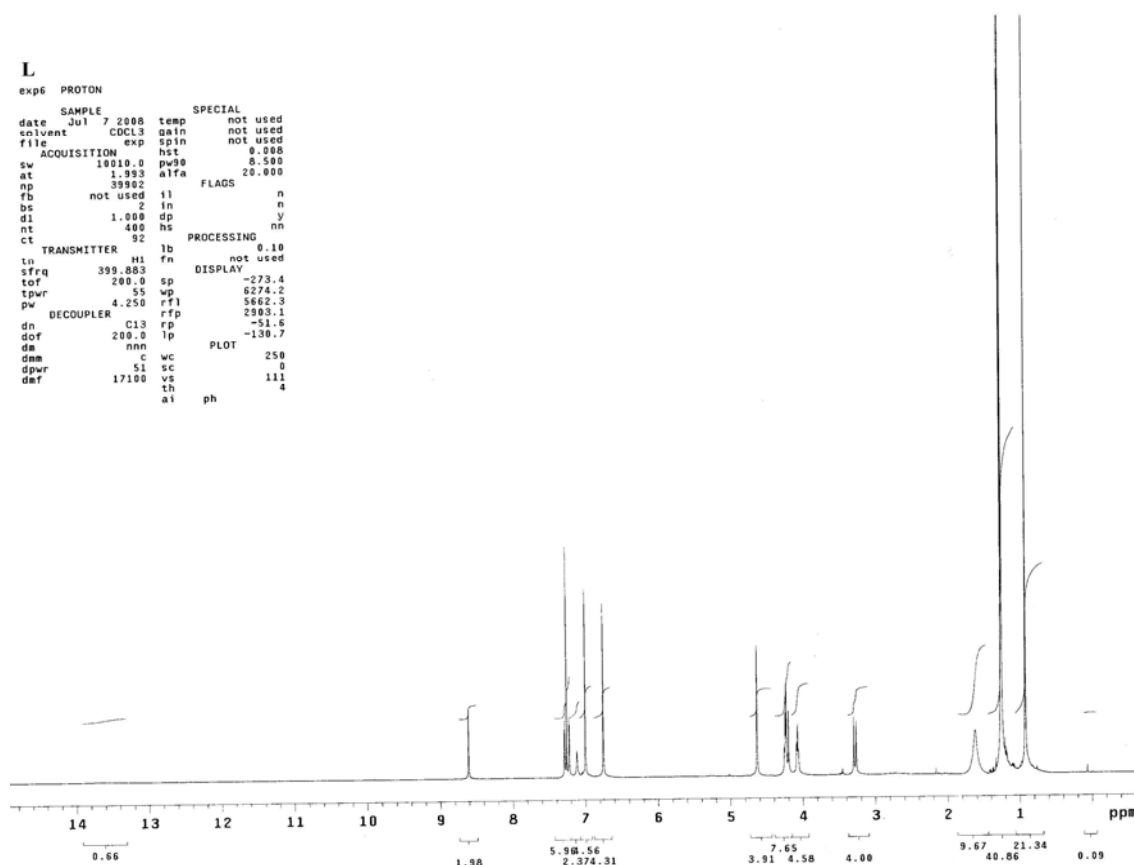
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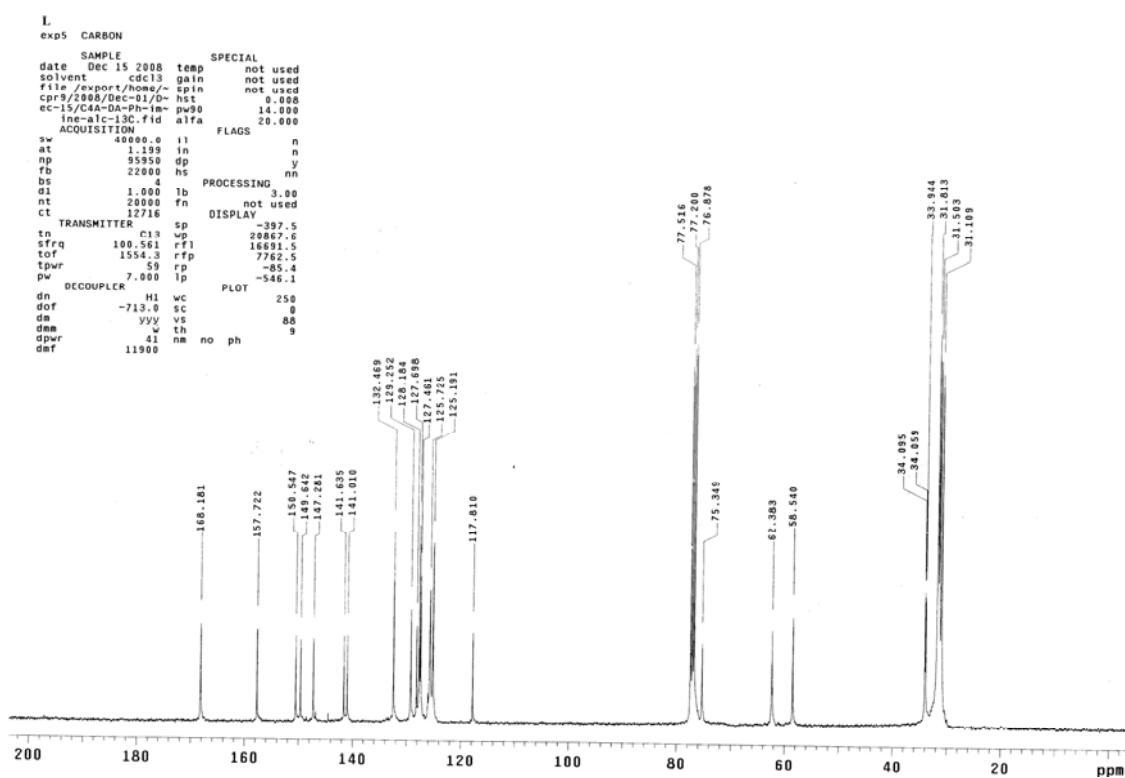
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S01. Spectral data of L

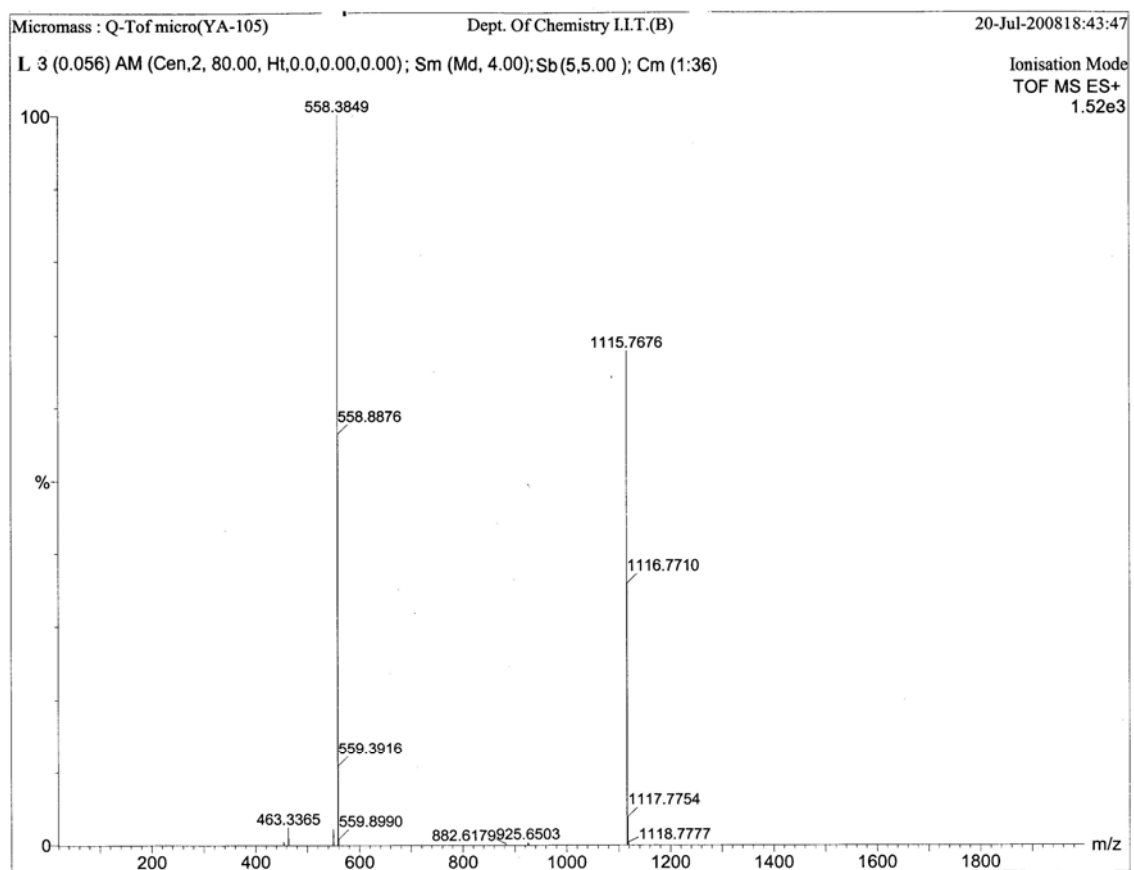
S01(a) ^1H NMR spectra of H_2L



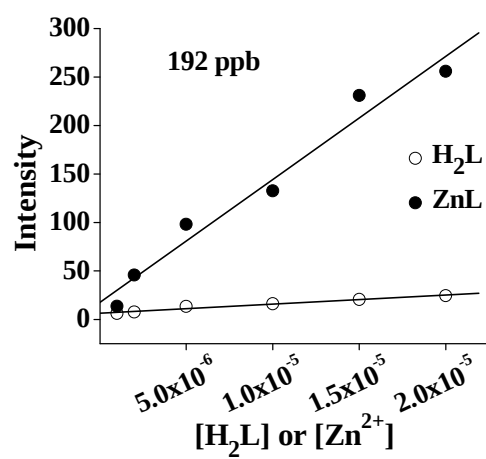
S01(b) ^{13}C NMR spectra of H_2L



S01(c) ESI MS spectra of H₂L



S02. Minimum detection limit calculation – H_2L with Zn^{2+} by keeping the ratio as 1:1.



S03: Computational data.

S03 (a) Cartesian coordinates of H₂L as obtained from B3LYP/6-31G level of optimization

Z	Cartesian coordinates			Z	Cartesian coordinates		
	x	y	z		x	y	z
6	-2.708221	0.038176	2.610400	1	0.595644	-1.230078	1.762177
6	-3.392020	1.262081	2.725928	1	-3.150823	4.878217	-2.212124
6	-3.364716	-1.197771	2.516476	6	-2.696049	1.367696	-2.734995
8	-1.286448	0.105651	2.541067	1	-1.723741	3.238994	-3.179730
6	-4.790945	1.226926	2.806877	1	-0.769062	2.142136	-2.173629
6	-2.645786	2.593277	2.677976	1	-4.432922	-4.497762	-2.421862
6	-4.766580	-1.186878	2.607950	6	-3.129185	-1.050900	-2.982879
6	-2.616816	-2.506921	2.262142	1	-3.089874	-3.098197	-3.636665
6	-0.594396	-0.066610	3.840002	1	-1.569221	-2.551819	-2.951613
1	-5.342184	2.158801	2.888091	6	4.056418	-1.293353	1.698988
6	-5.472917	0.007722	2.767122	6	2.450077	-2.526887	0.329641
6	-2.712936	3.255078	1.304993	6	-2.264799	0.033103	-2.743963
1	-3.091909	3.278577	3.406461	6	-4.045645	1.606271	-3.044204
1	-1.604031	2.448168	2.982159	6	-4.468420	-0.766752	-3.283127
1	-5.305667	-2.125198	2.528098	6	5.123543	-1.862023	0.975440
6	-3.047621	-3.148828	0.953336	8	4.347934	-0.421664	2.709959
1	-1.543940	-2.312873	2.244547	6	3.501857	-3.097516	-0.377935
1	-2.821055	-3.205614	3.083312	8	-0.902504	-0.278063	-2.452964
1	-0.538140	-1.138150	4.063735	6	-4.919480	0.555137	-3.331651
1	-1.195748	0.424591	4.613830	1	-4.414288	2.626729	-3.034858
6	0.790644	0.562937	3.789971	1	-5.157792	-1.586054	-3.462883
6	-2.086122	2.694022	0.170647	6	4.829781	-2.753463	-0.055544
6	-3.464034	4.430249	1.139443	6	-0.035422	-0.375573	-3.649494
6	-2.550683	-2.654120	-0.271861	1	5.665262	-3.167454	-0.609735
6	-3.997947	-4.176741	0.931378	1	0.079881	0.625684	-4.079361
1	0.707462	1.589358	3.405078	1	-0.531775	-1.020477	-4.384558
1	1.143152	0.651892	4.825652	6	1.309824	-0.970401	-3.260585
7	1.842077	-0.126946	3.043097	1	1.148362	-1.865921	-2.644737
6	-2.281980	3.251066	-1.111962	1	1.801506	-1.302829	-4.181212
8	-1.241757	1.593610	0.223067	7	2.250830	-0.077881	-2.578981
6	-3.604776	5.036339	-0.109602	6	1.925549	0.699743	-1.583334
1	-3.937900	4.872282	2.011592	1	3.717531	0.075357	-2.699495
6	-3.072163	-3.113209	-1.500762	6	2.955267	1.474165	-0.915277
8	-1.533556	-1.717595	-0.169271	1	0.900547	0.774490	-1.212622
1	-4.359509	-4.578795	1.873862	6	4.313188	1.329019	-1.309801
6	-4.486890	-4.683670	-0.276793	6	2.642943	2.329359	0.162135
6	1.610822	-0.978126	2.083825	6	5.345315	1.988739	-0.612968
1	3.458518	-0.076803	3.088544	8	4.635711	0.516533	-2.365253
6	-3.024534	4.432503	-1.229263	6	3.654126	3.002487	0.838733
6	-1.774623	2.524901	-2.348093	6	4.995527	2.815356	0.456679
1	-1.186164	1.111500	1.085563	1	5.782988	3.320275	1.009364
6	-4.037445	-4.133004	-1.477816	1	-5.956899	0.764864	-3.571206
6	-2.656199	-2.495387	-2.831685	1	-5.217789	-5.485235	-0.280804

1	-1.244660	-1.279482	-1.006500	1	-6.555657	-0.009949	2.837850
6	2.706683	-1.608044	1.372533	1	-4.171787	5.955404	-0.212436
1	3.305599	-3.806118	-1.176163				
1	1.416557	-2.769388	0.092602				
6	6.551653	-1.499265	1.338319				
1	6.880656	-2.105189	2.191257				
1	6.579955	-0.451924	1.664926				
8	7.490793	-1.754159	0.272064				
1	7.479098	-0.977583	-0.348318				
1	3.416661	3.655142	1.671309				
1	1.602778	2.439363	0.455824				
6	6.779810	1.788906	-1.055125				
1	7.473522	2.076656	-0.262852				
1	6.997147	2.406538	-1.939031				
8	7.081454	0.394712	-1.374867				
1	6.374306	0.090564	-1.995965				

S03 (b) Cartesian coordinates of [ZnL] as obtained from B3LYP/LanL2DZ level of optimization

Z	Cartesian coordinates			Z	Cartesian coordinates		
	x	y	z		x	y	z
6	-2.174277	0.182223	-2.717095	1	-3.597141	-4.826185	1.771623
6	-2.946389	-0.962402	-3.019384	6	-2.715924	-1.483033	2.643533
6	-2.716469	1.482011	-2.643427	1	-1.931485	-3.476758	2.924547
8	-0.803453	-0.040249	-2.386427	1	-0.861807	-2.386414	2.009271
6	-4.305621	-0.772550	-3.336249	1	-4.009268	4.487356	2.510027
6	-2.351181	-2.370464	-2.930126	6	-2.946387	0.961327	3.019493
6	-4.081232	1.626813	-2.974385	1	-2.768115	2.980154	3.739452
6	-1.901160	2.687255	-2.160252	1	-1.267040	2.329389	3.086879
6	0.157976	0.155230	-3.479745	6	3.183326	2.916635	-0.033129
1	-4.924203	-1.636392	-3.569233	6	3.123783	4.302450	-2.078450
6	-4.865106	0.517261	-3.333381	6	-2.174025	-0.183120	2.717164
6	-2.662837	-3.066582	-1.602412	6	-4.080640	-1.628145	2.974552
1	-2.767700	-2.981198	-3.739320	6	-4.305560	0.771165	3.336428
1	-1.266732	-2.330081	3.086859	6	3.672820	4.057177	0.686358
1	-4.536069	2.612889	-2.922274	8	3.024482	1.759046	0.632643
6	-2.447007	3.249921	-0.850980	6	3.617668	5.396638	-1.375970
1	-0.862511	2.385787	-2.009272	8	-0.803267	0.039683	2.386428
1	-1.932480	3.475911	-2.924473	6	-4.864751	-0.518773	3.333586
1	0.082277	1.192361	3.833585	1	-4.535251	-2.614325	2.922454
1	-0.097303	0.51666	4.3132980	1	-4.924323	1.634866	3.569445
6	1.564948	-0.165619	-2.970649	6	3.889919	5.259729	0.010184
6	-2.081817	-2.644335	-0.378053	6	0.158257	-0.155576	3.479702
6	-3.567043	-4.149107	1.574188	1	4.276319	6.114173	0.563833
6	-2.082375	2.643484	0.378139	1	0.082996	-1.192793	3.833384
6	-3.340227	4.335935	-0.833517	1	-0.097294	0.516094	4.313356
1	1.597542	-1.182646	-2.571653	6	1.565100	0.165915	2.970653

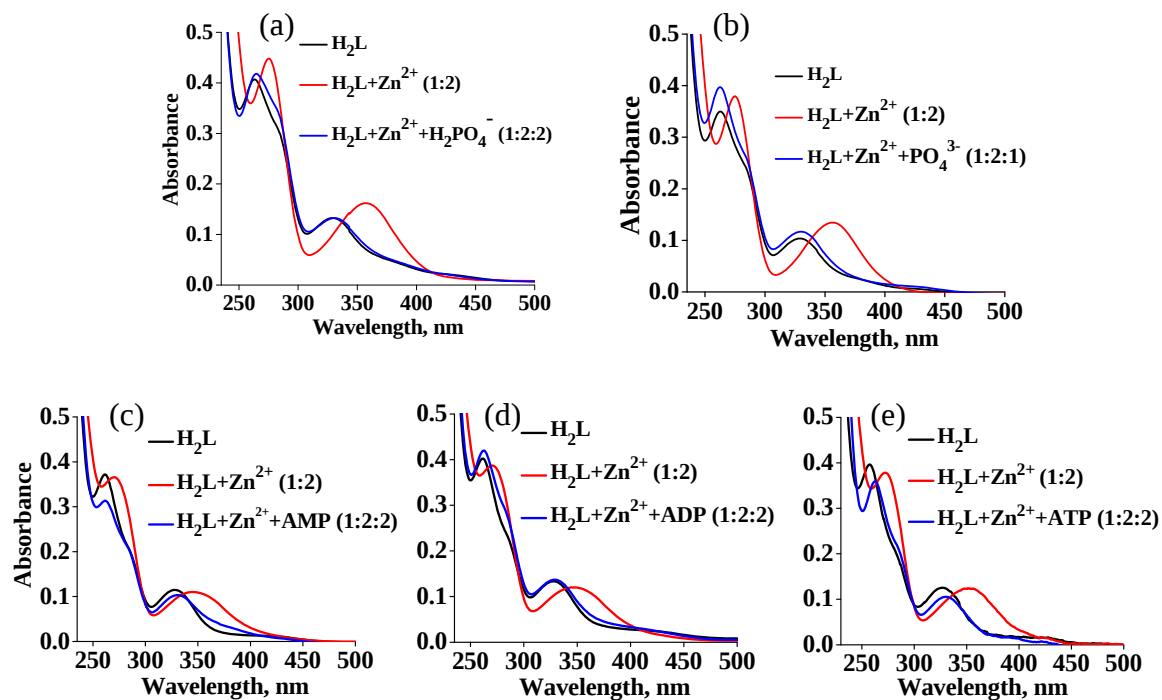
1	2.248352	-0.129745	-3.833095	1	1.597264	1.182985	2.571726
7	2.042593	0.755247	-1.900115	1	2.248498	0.130275	3.833114
6	-2.446182	-3.250890	0.851083	7	2.043158	-0.754674	1.900069
8	-1.123720	-1.644211	-0.285913	6	2.378178	-1.976001	2.257859
6	-3.896587	-4.798485	-0.372910	6	2.892534	-3.048276	1.434165
1	-4.008349	-4.488726	-2.509820	1	2.274897	-2.242527	3.319347
6	-2.663426	3.065580	1.602535	6	3.184990	-2.915398	0.032990
8	-1.123998	1.643630	0.285958	6	3.126527	-4.301223	2.078338
1	-3.598472	4.824880	-1.771451	6	3.675102	-4.055648	-0.686538
6	-3.897742	4.797129	0.373105	8	3.025347	-1.757920	-0.632776
6	2.376836	1.976778	-2.257925	6	3.621004	-5.395116	1.375815
6	-3.339104	-4.337157	0.833675	6	3.893013	-5.258059	-0.010374
6	-1.900382	-2.688102	2.160317	1	4.279877	-6.112274	-0.564052
1	-0.947953	-1.091094	-1.095803	1	-5.913271	-0.656403	3.586017
6	-3.567933	4.147854	1.574367	1	-4.580582	5.642559	0.375941
6	-2.351509	2.369528	2.930222	1	-5.913669	0.654652	3.585762
1	-0.948053	1.090564	1.095842	1	-4.579197	-5.644102	-0.375705
6	2.890631	3.049352	-1.434268	30	2.373005	0.000396	-0.000031
1	2.273276	2.243264	-3.319395	1	3.799446	-6.341878	1.877020
1	2.910320	-4.390545	3.142386				
1	3.795470	6.343516	-1.877184				
1	2.907402	4.391653	-3.142473				
6	3.918577	-3.927410	-2.181908				
1	2.949456	-3.917796	-2.712176				
1	4.496949	-4.781291	-2.548498				
8	4.682802	-2.735743	-2.542819				
1	4.265055	-1.989866	-2.045716				
6	3.916544	3.929078	2.181701				
1	2.947491	3.918930	2.712084				
1	4.494478	4.783288	2.548216				
8	4.681478	2.737843	2.542531				
1	4.264088	1.991724	2.045487				

S03 (c) Cartesian coordinates of [CdL] as obtained from B3LYP/LanL2DZ level of optimization

6	-2.416435	-1.668501	-2.289503	1	-0.053755	-4.723708	3.500347
6	-2.478867	-3.058022	-2.039831	6	-1.170501	-1.212358	3.156210
6	-3.555314	-0.851945	-2.440072	1	0.423322	-2.490392	3.870130
8	-1.119542	-1.092333	-2.221057	1	0.885319	-1.449317	2.523116
6	-3.749697	-3.663572	-2.017847	1	-5.133373	3.162766	1.986909
6	-1.202146	-3.855108	-1.757042	6	-2.416802	0.899041	2.806708
6	-4.808921	-1.501942	-2.419891	1	-2.924720	3.003288	2.912131
6	-3.464236	0.673264	-2.559144	1	-1.523642	2.635334	1.892939
6	-0.349677	-0.875284	-3.455314	6	0.924662	3.509188	-0.867286
1	-3.831862	-4.731357	-1.827288	6	1.859321	4.253779	-3.033982
6	-4.907281	-2.890648	-2.223878	6	-1.226339	0.143163	2.767345
6	-0.868956	-4.045549	-0.270493	6	-2.332788	-1.786258	3.708601
1	-1.314738	-4.852645	-2.196198	6	-3.557681	0.287844	3.368361
1	-0.350968	-3.386388	-2.264051	6	0.966880	4.881143	-0.435489
1	-5.713472	-0.909449	-2.535125	8	0.444086	2.570759	-0.039294
6	-3.939587	1.403089	-1.302591	6	1.887216	5.581824	-2.605436
1	-2.427616	0.960439	-2.747446	8	-0.036137	0.754192	2.272534
1	-4.078160	0.998514	-3.409703	6	-3.512157	-1.033919	3.840938
1	-0.841350	-0.081609	-4.032850	1	-2.317690	-2.831300	4.009312
1	-0.340590	-1.801915	-4.047527	1	-4.490614	0.845160	3.407753
6	1.082944	-0.480863	-3.071414	6	1.430389	5.881490	-1.302277
6	-0.484062	-2.984988	0.593609	6	0.853727	1.278490	3.337817
6	-0.929125	-5.350359	0.265324	1	1.431285	6.916390	-0.959687
6	-3.032098	1.656563	-0.245022	1	1.087765	0.452765	4.023755
6	-5.271434	1.842991	-1.163682	1	0.321427	2.067610	3.883939
1	1.592727	-1.286627	-2.535569	6	2.123549	1.841823	2.684155
1	1.635803	-0.315234	-4.011403	1	1.869306	2.763936	2.151485
7	1.090852	0.728614	-2.212439	1	2.841106	2.093032	3.485037
6	-0.217310	-3.220940	1.964856	7	2.664328	0.857220	1.729109
8	-0.366735	-1.663022	0.145721	6	3.900118	0.439297	1.828926
6	-0.625200	-5.610474	1.610316	6	4.564030	-0.559344	1.008790
1	-1.210767	-6.171324	-0.391432	1	4.532969	0.868707	2.622676
6	-3.461511	2.246189	0.971353	6	3.891479	-1.338193	-0.015405
8	-1.710106	1.264134	-0.422313	6	5.944046	-0.791104	1.275831
1	-5.972202	1.685807	-1.982076	6	4.673940	-2.335693	-0.716876
6	-5.699190	2.499780	0.004319	8	2.615967	-1.197394	-0.317028
6	1.378103	1.868336	-2.782930	6	6.680368	-1.750857	0.583039
6	-0.277850	-4.540064	2.451220	6	6.024436	-2.523961	-0.408133
6	0.075779	-2.068565	2.917660	1	6.584534	-3.292482	-0.941665
1	-0.666070	-1.487796	-0.804072	1	-4.399825	-1.485921	4.276803
6	-4.797306	2.683854	1.068482	1	-6.723837	2.853227	0.088478
6	-2.522551	2.293072	2.177904	1	-5.885014	-3.366100	-2.210872
1	-0.994698	1.956354	-0.206613	1	-0.663407	-6.625597	1.996263
6	1.389397	3.204256	-2.196778	1	7.731080	-1.914291	0.804520
1	1.652588	1.855646	-3.850239	1	6.428486	-0.195319	2.050175
1	2.242628	6.370679	-3.261856				

1	2.201108	4.004589	-4.038363				
6	3.996773	-3.183682	-1.764573				
1	2.983742	-3.446392	-1.451491				
1	4.576197	-4.100746	-1.948486				
8	3.794257	-2.482805	-3.058604				
1	4.618625	-2.003358	-3.288970				
6	0.511807	5.240338	0.958013				
1	-0.306639	4.597067	1.283545				
1	0.191611	6.291568	1.000737				
8	1.561529	5.016162	1.982920				
1	2.388330	5.461570	1.698459				
48	1.060170	0.335140	0.131780				

S04. Absorption spectral traces obtained during the titration of [ZnL] (2:1) with different phosphates and nucleotides (a) H_2PO_4^- , (b) PO_4^{3-} , (c) AMP, (d) ADP and (e) ATP.



Instrumental Details. ^1H and ^{13}C NMR spectra were measured on an NMR spectrometer working at 400 MHz. The mass spectra were recorded on micromass equipment using the electrospray ionization method. Steady-state fluorescence spectra were measured on Perkin-Elmer LS55. The absorption spectra were measured on JASCO V570. The elemental analyses were performed on ThermoQuest microanalysis, and the FT IR spectra were measured on Perkin-Elmer spectrometer using KBr pellets.