

Supporting information

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Comparative analysis of Zn(II)-Complexes as model metalloenzyme for mimicking Jack Bean Urease

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NMR

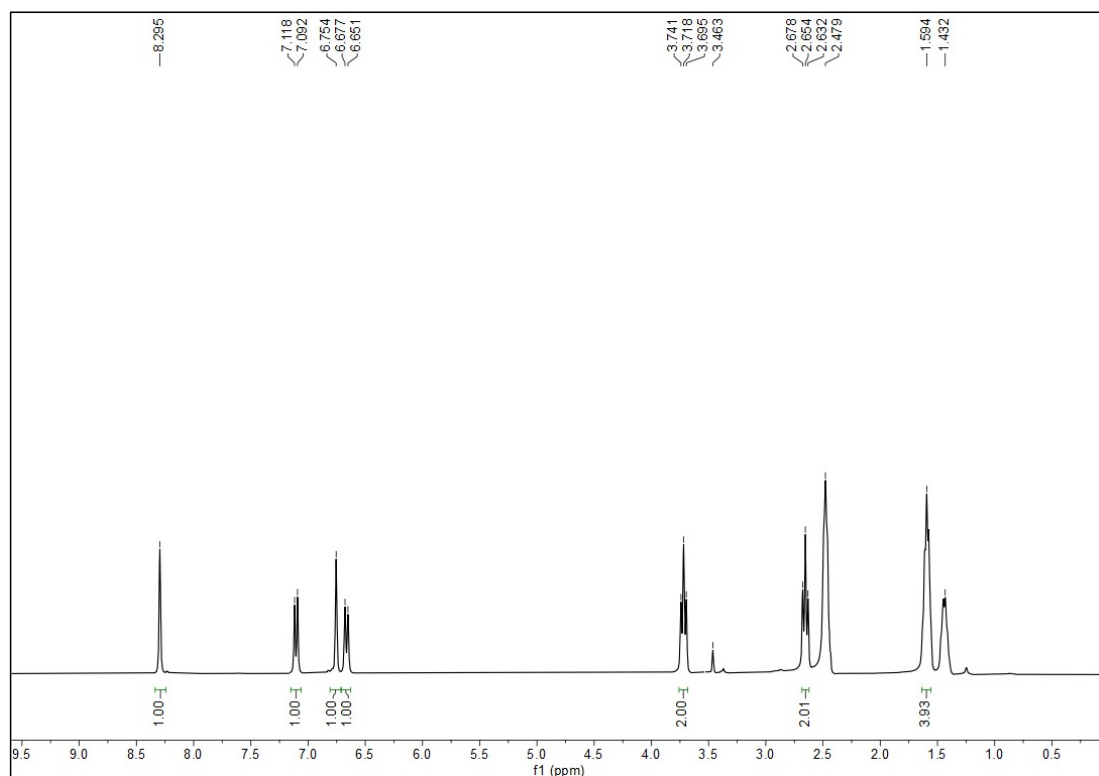


Fig. S1. ¹H NMR spectrum of ligand HL¹

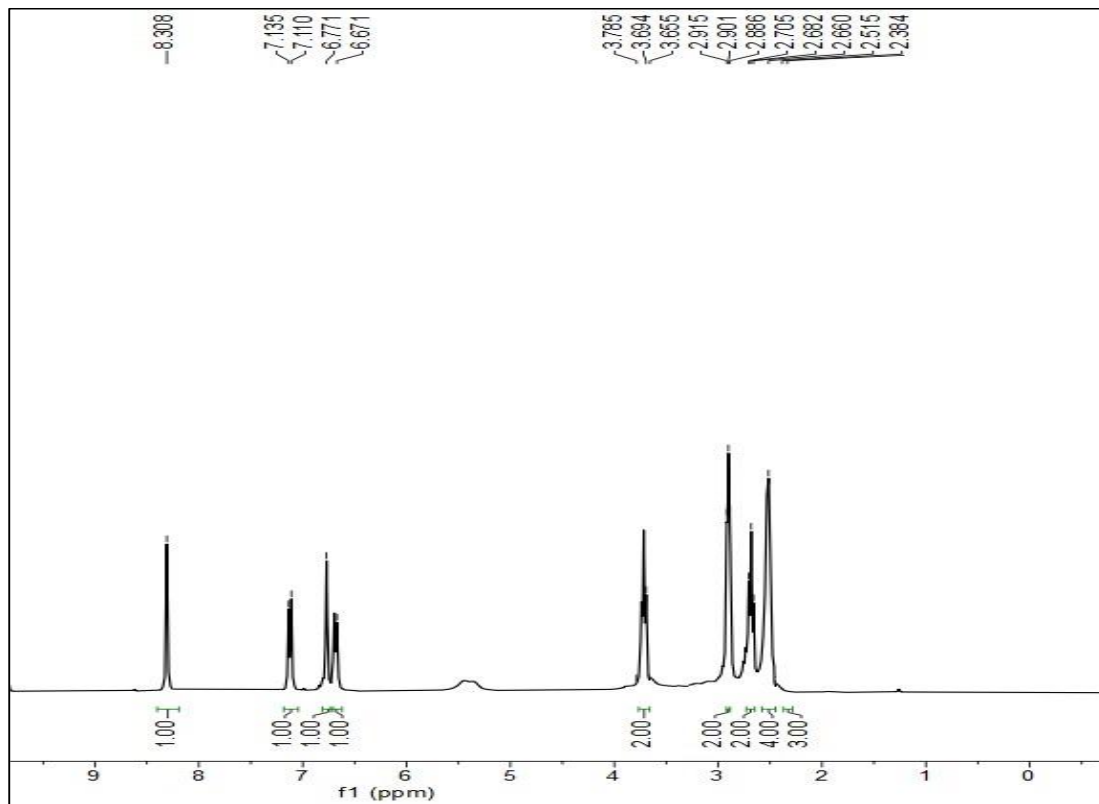


Fig. S2. ¹H NMR spectrum of ligand HL²

FT-IR:

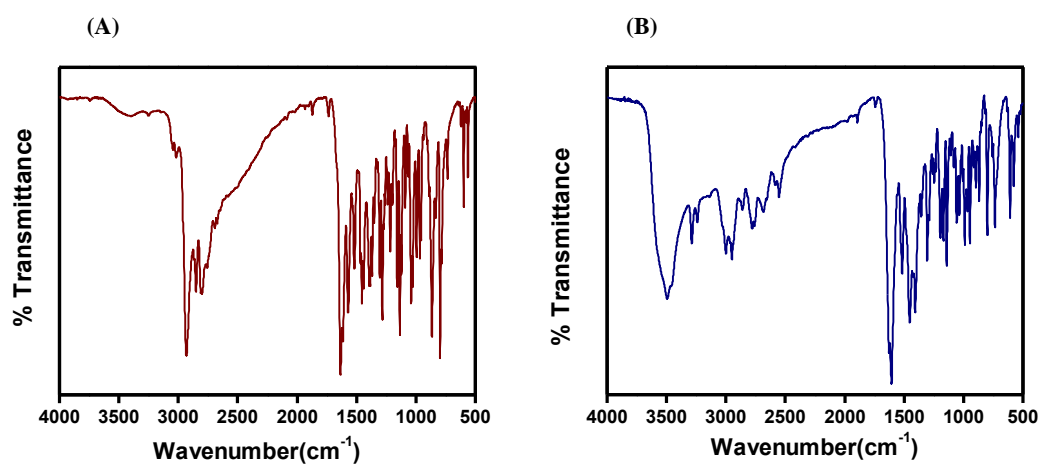


Fig. S3. FT-IR spectrum of (A) HL¹, (B) PPR-HMB-Zn

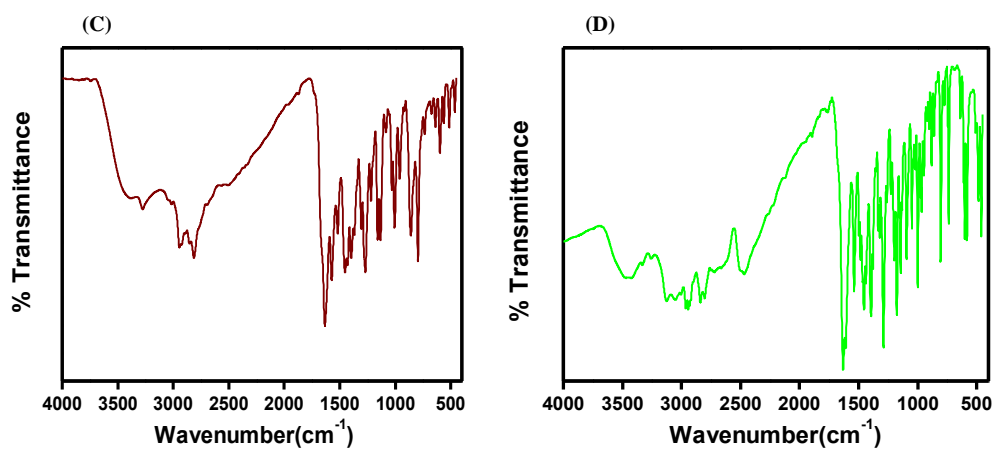


Fig. S4. FT-IR spectrum of (C) HL², (D) PZ-HMB-Zn

UV-Vis

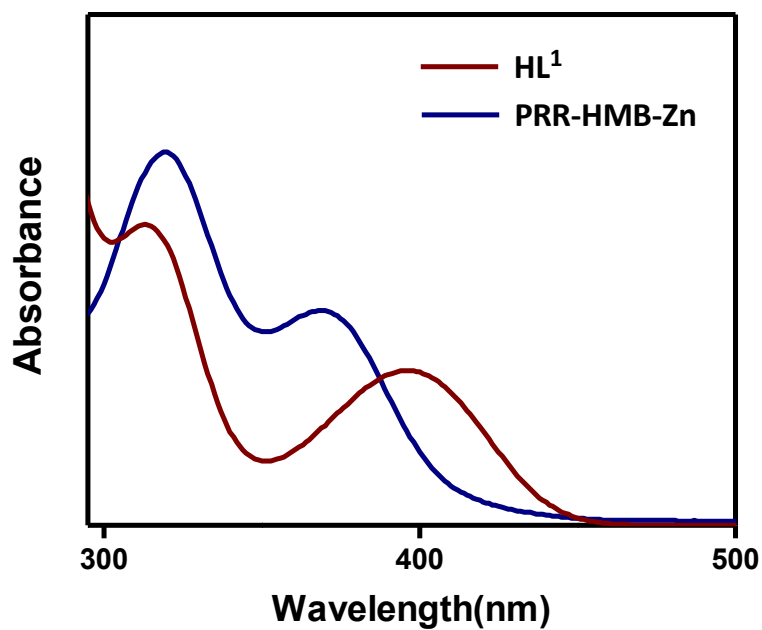


Fig. S5. UV-vis spectrum of ligand HL¹ and **PRR-HMB-Zn** complex

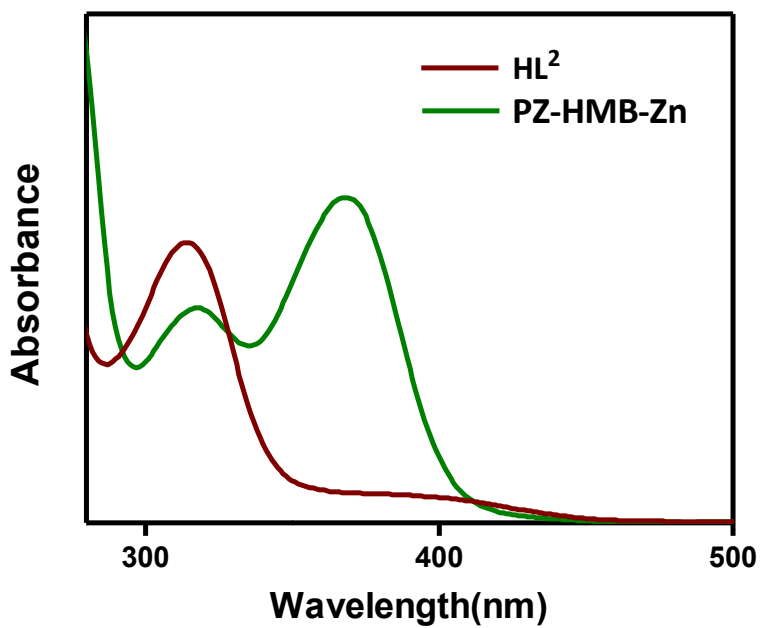


Fig. S6. UV-vis spectrum of ligand HL² and **PZ-HMB-Zn** complex

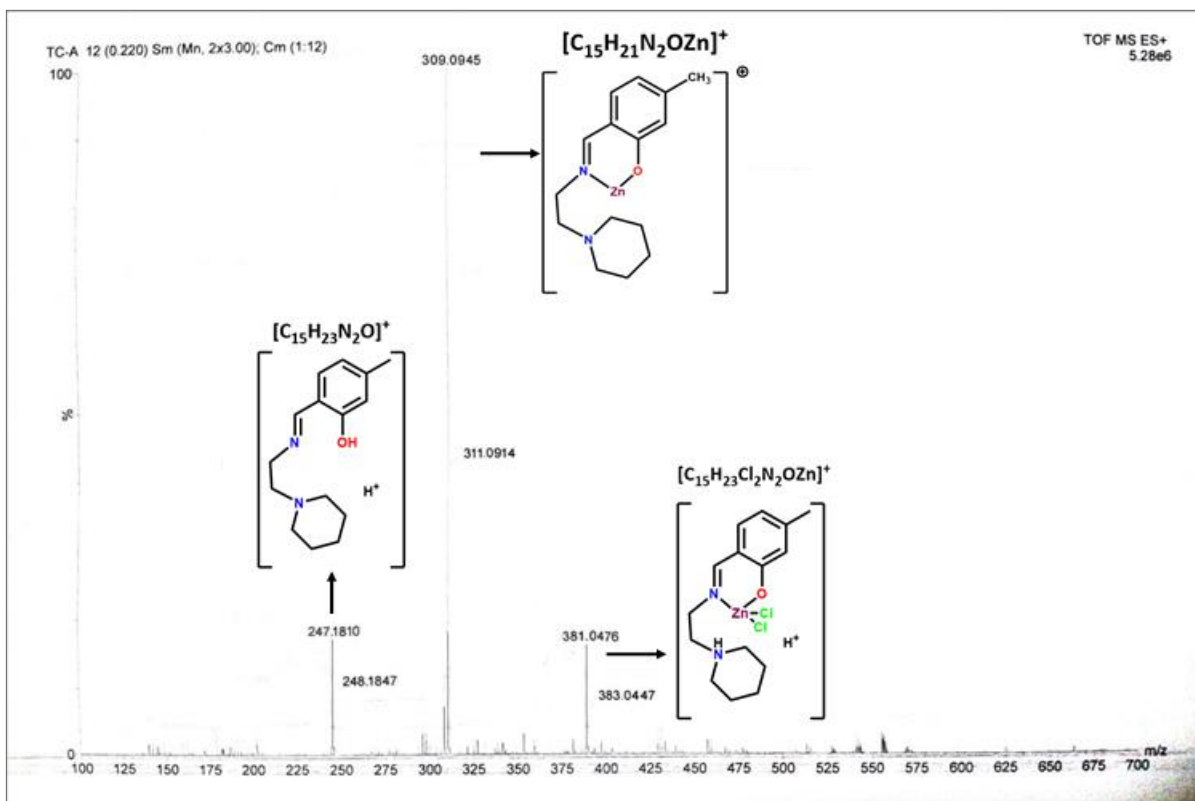


Fig. S7. ESI-MS spectra of PPR-HMB-Zn complex

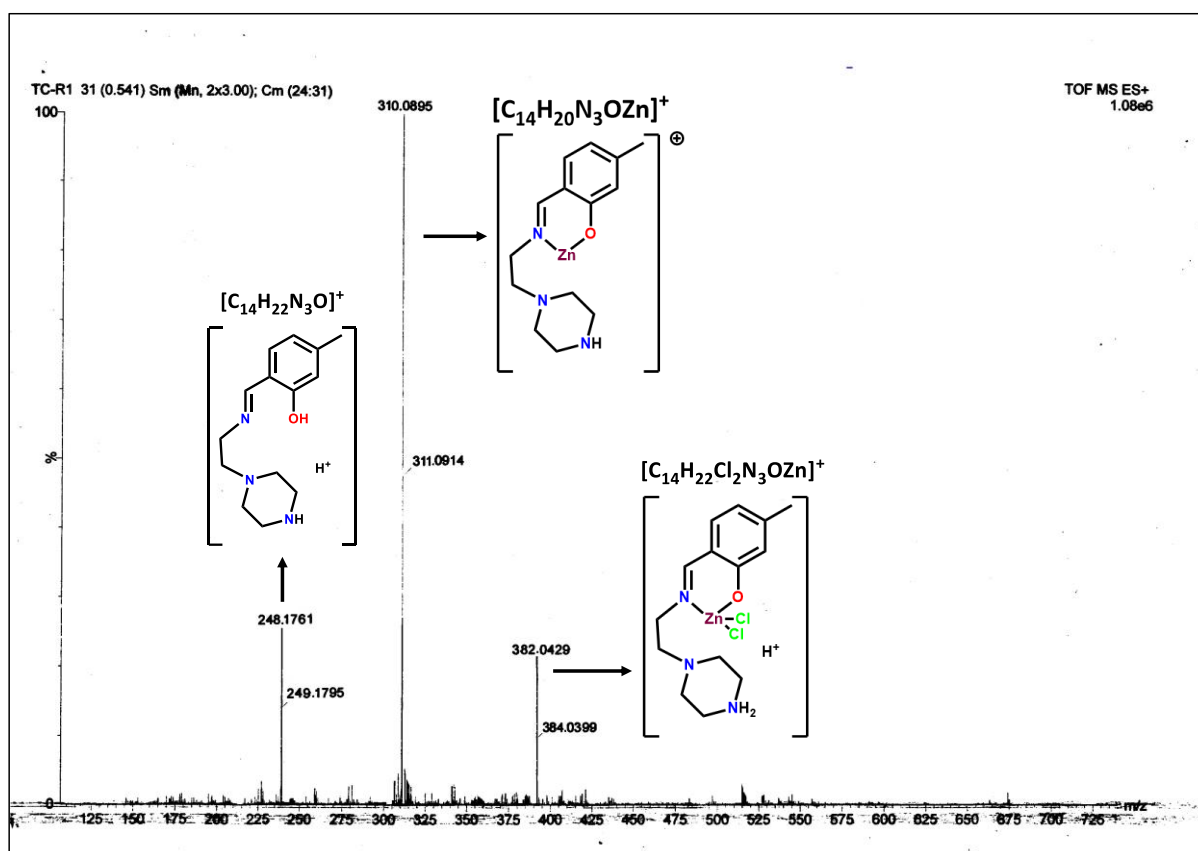


Fig. S8. ESI-MS spectra of PZ-HMB-Zn complex

Phosphatase activity of PZ-HMB-Zn:

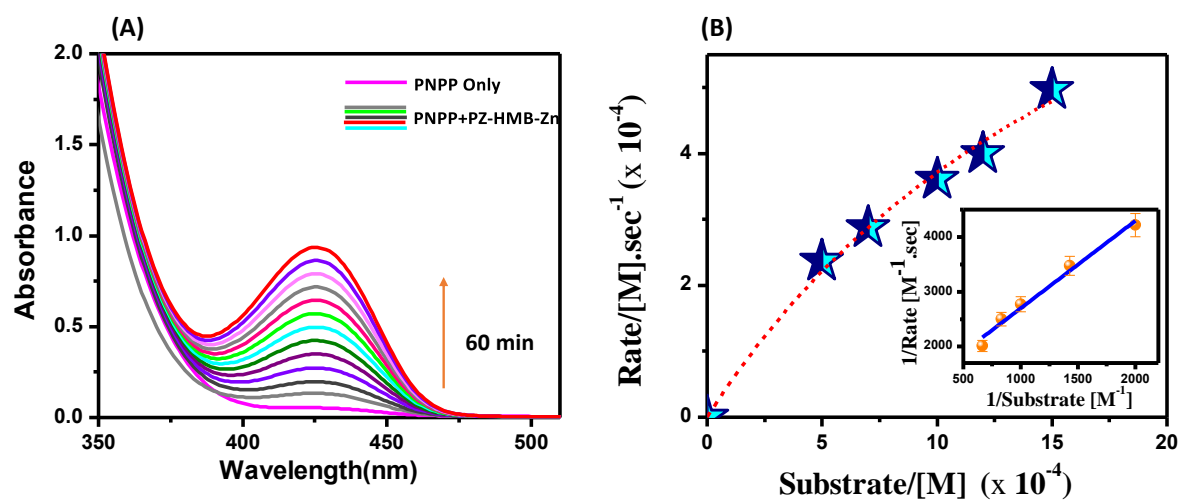
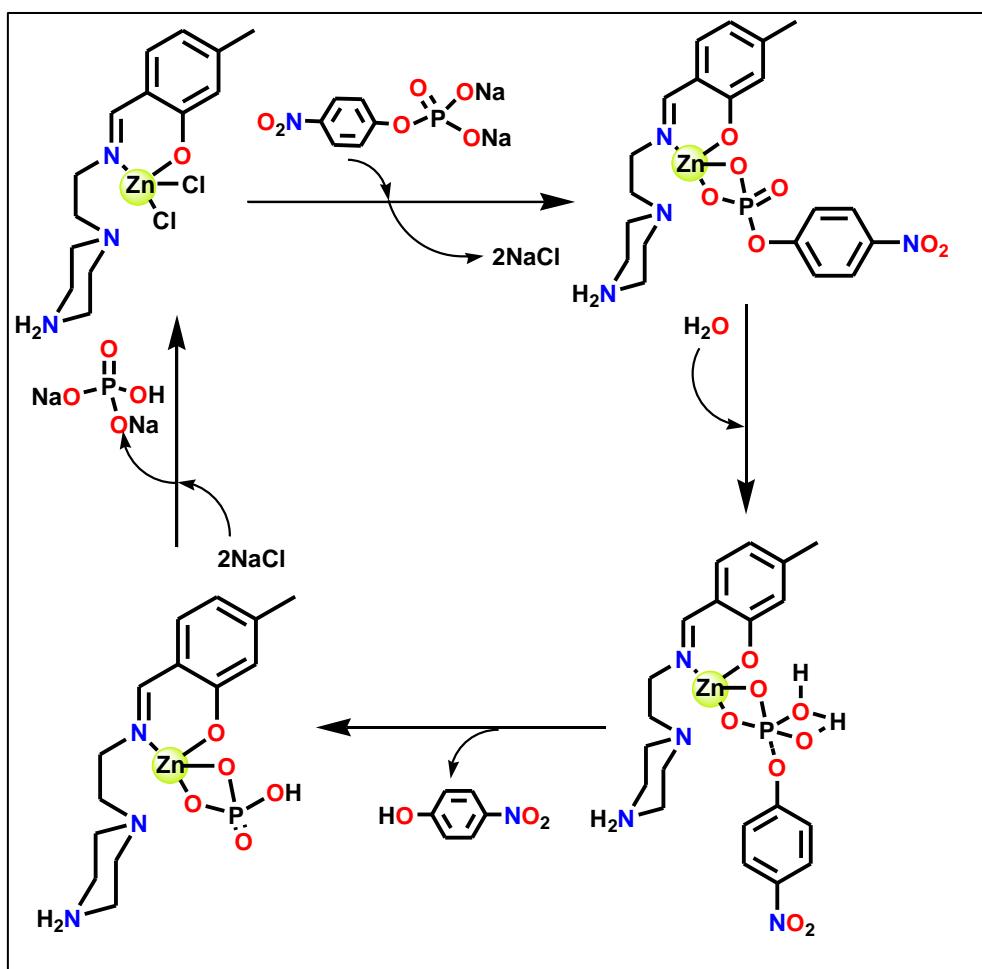


Fig. S9. (A) Time dependent wavelength scan for the hydrolysis of PNPP in the presence of **PZ-HMB-Zn** complex recorded at 25⁰C at intervals of 5 min (B) Michaelis-Menten kinetics plot attained from absorption profile of PNPP adding **PZ-HMB-Zn** Complex owing to the accumulation of p-nitrophenolate ($\lambda_{\max}= 425\text{nm}$). Inset shows Lineweaver-Burk plot, slope = 1.59768, intercept =1101.293, $R^2= 0.97838$.

Mechanism of Phosphatase activity for PZ-HMB-Zn:



Scheme S1. Plausible mechanistic aspect of **PZ-HMB-Zn** complex mediated hydrolytic cleavage of P-O bond of 4-NPP.

Urease activity of PZ-HMB-Zn:

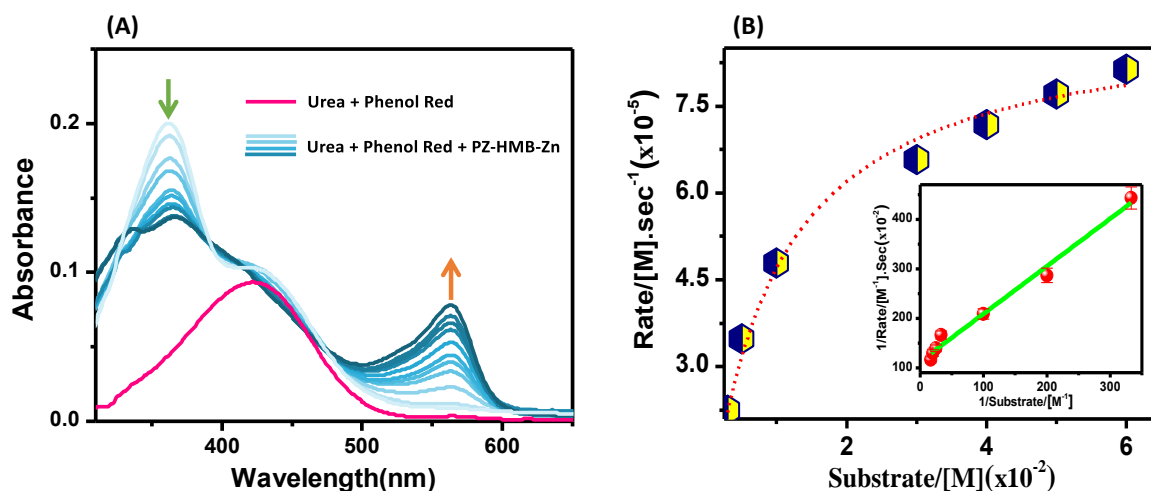


Fig. S10. (A) Typical UV-metric wavelength scan of phenol red recorded during a kinetic run for the **PZ-HMB-Zn** catalyzed hydrolysis of urea (B) Michaelis-Menten kinetics plot attained from absorption profile of phenol red recorded at 563 nm for the hydrolysis of urea with catalytic addition of **PZ-HMB-Zn**; inset shows Lineweaver-Burk plot, slope = 96.208, intercept = 11276, $R^2 = 0.9844$.

Mechanism for PZ-HMB-Zn:

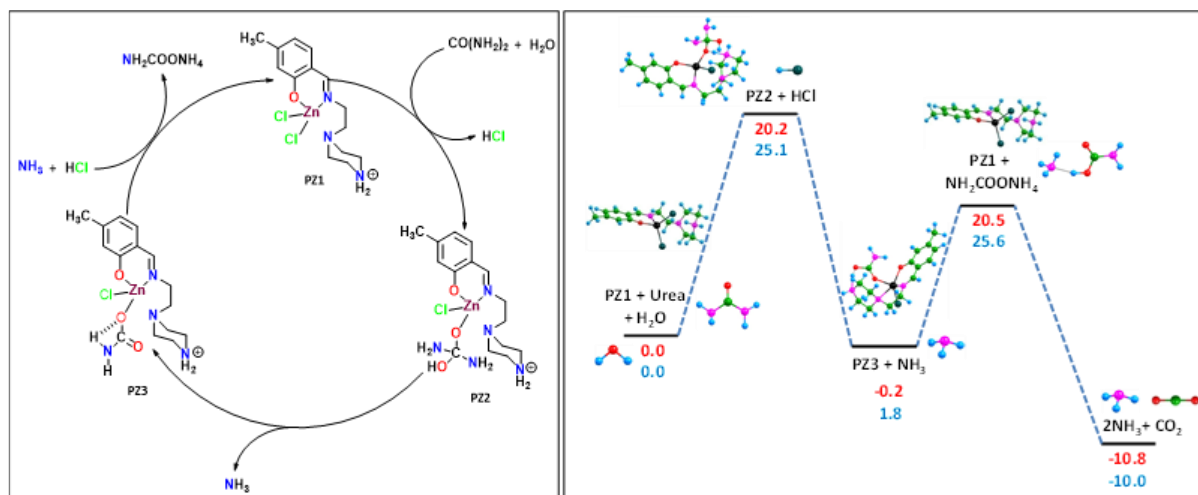


Fig. S11. Left panel: DFT supported plausible mechanism for the catalytic involvement of **PZ-HMB-Zn** in urea hydrolysis; Right panel: associated energy profile diagram for the catalysis mechanism carried out using functionals TPSSH (top) and B3LYP (bottom).

Table S1. Bond Lengths (Å) for Complex **PPR-HMB-Zn**.

		Length/Å			Length/Å
Zn1	Cl1	2.225(2)	C2	C7	1.402(10)
Zn1	Cl2	2.284(2)	C3	C4	1.388(11)
Zn1	N1	2.047(6)	C4	C5	1.423(11)
Zn1	O1	1.963(5)	C5	C6	1.443(10)
N1	C8	1.293(10)	C5	C8	1.448(10)
N1	C9	1.474(9)	C6	C7	1.434(10)
N2	C10	1.506(9)	C9	C10	1.535(10)
N2	C11	1.515(9)	C11	C12	1.524(11)
N2	C15	1.492(10)	C12	C13	1.518(12)
O1	C6	1.330(9)	C13	C14	1.529(12)
C1	C2	1.522(10)	C14	C15	1.533(11)

Table S2. Bond Angles (°) for Complex **PPR-HMB-Zn**.

		Angle/°			Angle/°		
Cl1	Zn1	Cl2	113.82(8)	C3	C4	C5	122.3(7)
N1	Zn1	Cl1	110.01(19)	C4	C5	C6	118.2(6)
N1	Zn1	Cl2	110.42(18)	C4	C5	C8	115.7(7)
O1	Zn1	Cl1	117.84(16)	C8	C5	C6	125.9(6)
O1	Zn1	Cl2	108.49(16)	O1	C6	C5	123.9(6)
O1	Zn1	N1	94.6(2)	O1	C6	C7	117.8(6)
C8	N1	Zn1	120.2(5)	C7	C6	C5	118.3(6)
C8	N1	C9	117.5(6)	C2	C7	C6	121.2(7)

	Angle/°		Angle/°
C9 N1 Zn1	122.2(5)	N1 C8 C5	126.2(7)
C10 N2 C11	109.6(6)	N1 C9 C10	110.1(6)
C15 N2 C10	112.3(6)	N2 C10 C9	110.8(6)
C15 N2 C11	112.1(5)	N2 C11 C12	110.2(6)
C6 O1 Zn1	121.9(4)	C13C12 C11	111.4(7)
C3 C2 C1	120.4(7)	C12C13 C14	109.9(7)
C3 C2 C7	120.2(7)	C15C14 C13	111.9(7)
C7 C2 C1	119.5(7)	N2 C15 C14	110.9(7)
Cl1 Zn1 Cl2	113.82(8)	C3 C4 C5	122.3(7)

Table S3. Selected hydrogen bonding distances (Å) and angles (°) for PPR-HMB-Zn

D-H....A	D-H (Å)	D....A (Å)	A...H (Å)	<D-HA(deg)
N2--H2..O2	1.0000	1.7800	2.776	174.00
O2—H11..O1	0.9300	1.8500	2.772	180.00
O2—H12..Cl2	0.8500	2.4300	3.236	160.00
C11--H11A..O2	0.9900	2.5100	3.416	153.00

Table S4. Bond Lengths (Å) for Complex PZ-HMB-Zn.

	Length/Å		Length/Å
Zn1 Cl1	2.2636(9)	C1 C2	1.509(4)
Zn1 Cl2	2.2300(9)	C2 C3	1.398(4)
Zn1 N1	2.004(3)	C2 C7	1.387(4)
Zn1 O1	1.956(2)	C3 C4	1.374(4)
N1 C8	1.291(4)	C4 C5	1.406(4)

	Length/Å		Length/Å
N1 C9	1.464(4)	C5 C6	1.424(4)
N2 C10	1.458(4)	C5 C8	1.448(4)
N2 C11	1.463(3)	C6 C7	1.396(4)
N2 C14	1.470(4)	C9 C10	1.529(4)
N3 C12	1.489(4)	C11 C12	1.508(4)
N3 C13	1.492(4)	C13 C14	1.513(4)
O1 C6	1.337(3)		

Table S5. Bond Angles (°) for Complex **PZ-HMB-Zn**.

Angle/°				Angle/°			
C12	Zn1	C11	108.82(4)	C4	C3	C2	119.6(3)
N1	Zn1	C11	113.10(8)	C3	C4	C5	122.6(3)
N1	Zn1	C12	113.72(8)	C4	C5	C6	118.0(3)
O1	Zn1	C11	112.73(7)	C4	C5	C8	116.1(3)
O1	Zn1	C12	112.96(7)	C6	C5	C8	125.7(3)
O1	Zn1	N1	95.10(9)	O1	C6	C5	123.1(3)
C8	N1	Zn1	119.5(2)	O1	C6	C7	118.6(3)
C8	N1	C9	118.8(3)	C7	C6	C5	118.3(3)
C9	N1	Zn1	121.66(19)	C2	C7	C6	122.7(3)
C10	N2	C11	109.2(2)	N1	C8	C5	126.8(3)
C10	N2	C14	111.4(2)	N1	C9	C10	110.2(3)
C11	N2	C14	108.0(2)	N2	C10	C9	111.3(2)
C12	N3	C13	111.6(2)	N2	C11	C12	111.2(2)
C6	O1	Zn1	121.15(18)	N3	C12	C11	111.0(2)

Angle/°				Angle/°			
C3	C2	C1	120.4(3)	N3	C13	C14	110.9(2)
C7	C2	C1	120.7(3)	N2	C14	C13	110.1(3)
C7	C2	C3	118.8(3)				

Table S6. Selected hydrogen bonding distances (Å) and angles (°) for PZ-HMB-Zn

D-H...A	D-H (Å)	D...A (Å)	A...H (Å)	<D-HA(deg)
N3--H3A..C11	0.8600	2.5900	3.291	140.00
N3--H3B..O1	0.9800	1.7400	2.708	169.00
C7--H7..C11	0.9500	2.7600	3.683	163.00
C12--H12A..C12	0.9900	2.6700	3.634	165.00

Table S7. Kinetic parameters of Lineweaver-Burk plot for Phosphatase and Urease activity of both the complexes PPR-HMB-Zn and PZ-HMB-Zn

Kinetic parameters of Lineweaver Burk Plot					
Activity	Material	V _{max} (M S ⁻¹)	K _M (M)	K _{cat} (S ⁻¹)	K _{cat} / K _M
Phosphatase	PPR-HMB-Zn	1×10 ⁻³	1×10 ⁻³	20	20×10 ³
	PZ-HMB-Zn	9.3×10 ⁻⁴	1.8×10 ⁻³	18.6	10.333×10 ³
Urease	PPR-HMB-Zn	1.4×10 ⁻⁴	1.8×10 ⁻²	2.81	1.50×10 ²
	PZ-HMB-Zn	9.08×10 ⁻⁵	0.93×10 ⁻²	1.82	1.95×10 ²

Table S8. Comparison of kinetic parameters between our synthesized complexes to the literature survey for phosphatase-like activity

Kinetic parameters of Phosphatase-like Activity						
	Material	V_{max} ($M S^{-1}$)	$K_M(M)$	K_{cat} (S^{-1})	K_{cat}/ K_M	Std. error
Our Work	PPR-HMB-Zn	1.04×10^{-3}	1.15×10^{-3}	20.8	18.086×10^3	0.24503
	PZ-HMB-Zn	9.1×10^{-4}	1.4×10^{-3}	18.2	13×10^3	0.35807
Reference (41)	Compound 1	9.6097×10^{-4}	7.905×10^{-4}	38.436	48.6×10^3	0.03664
	Compound 2	7.2397×10^{-4}	6.8116×10^{-4}	28.959	42.5×10^3	0.07266
Reference (44)	Complex 2	4.927×10^{-4}	1.451×10^{-3}	4.927	3.395×10^3	0.35807
	Complex 3	1.5505×10^{-3}	3.0944×10^{-3}	15.5056	5.010×10^3	0.24053
	Complex 4	8.715×10^{-4}	2.25×10^{-3}	8.7155	3.873×10^3	0.21863
	Complex 5	6.6332×10^{-4}	4.8262×10^{-3}	6.6332	1.374×10^3	0.31941
Reference (45)	Complex 1	8.07×10^{-4}	1.63×10^{-3}	16.15	9.98×10^3	0.16
	Complex 2	6.26×10^{-4}	1.56×10^{-3}	12.52	8.02×10^3	0.15
	Complex 3	4.56×10^{-4}	2.27×10^{-3}	9.116	3.99×10^3	0.19
Reference (46)	Complex 1	8.326×10^{-4}	8.8426×10^{-4}	17.6527	19.963×10^3	0.000263
	Complex 2	3.264×10^{-4}	6.4087×10^{-4}	6.5295	10.188×10^3	0.000106
	Complex 3	8.210×10^{-4}	10.911×10^{-4}	16.4204	15.049×10^3	0.00836
	Complex 4	11.930×10^{-4}	12.452×10^{-4}	23.8780	19.176×10^3	0.000012

Coordinates of the optimized complexes.

1a

C	-3.31208600	-1.83421200	1.06959300
C	-2.41121000	-0.78034100	0.74133000
C	-2.83559700	0.22274700	-0.20936200
C	-4.14892600	0.08991600	-0.75281000
C	-4.99872500	-0.94995100	-0.42115100
C	-4.56529200	-1.93349300	0.51039500
H	-2.98824400	-2.58016000	1.79357900
H	-4.45532200	0.85553200	-1.45962700
H	-5.22637800	-2.75159800	0.78218300
O	-2.11183900	1.23231400	-0.57890100
C	-1.16200700	-0.77008300	1.44030000
H	-1.07710300	-1.54880700	2.21337500
N	-0.14771800	0.03921900	1.29284300
C	0.93833400	-0.08113700	2.25866200
H	0.93969500	-1.07391300	2.73422100
H	0.78733800	0.65110800	3.06503700
C	2.31341100	0.26596100	1.68615500
H	3.07254700	0.12971000	2.46338000
H	2.31856700	1.31246400	1.36603100
Zn	-0.19453600	1.51176500	-0.27741600
C	4.12591500	-0.07511500	0.04901700
C	2.71182600	-2.02796300	0.70251300
H	2.10595000	-0.30548100	-0.31975600
C	4.60338000	-0.81890900	-1.19745200
H	4.80039100	-0.23971500	0.89729500
H	4.04206500	0.99883000	-0.13232600
C	3.17353700	-2.78117800	-0.54674600
H	3.35295500	-2.24716100	1.56494300
H	1.68307600	-2.28812700	0.95503200
C	4.57414800	-2.33918500	-0.99054300
H	5.61666800	-0.47088200	-1.42618300
H	3.96652800	-0.53926300	-2.04377200
H	3.14997800	-3.85292300	-0.32052300
H	2.45204200	-2.60587700	-1.35344400
H	4.85354500	-2.85154700	-1.91678900
H	5.31445000	-2.62949200	-0.23107600
N	2.75619800	-0.53988400	0.48953500
Cl	0.90834900	3.36798100	0.48817000
Cl	1.10341000	0.32585900	-1.92762100
C	-6.37675200	-1.05363600	-1.02893500
H	-6.57577900	-0.22867500	-1.71796100
H	-6.49161400	-1.99445000	-1.58104700
H	-7.14956900	-1.04218300	-0.25066700

2a

C	-3.64173300	2.15664400	-0.43682000
C	-2.69884200	1.09428300	-0.49781100
C	-3.04784800	-0.17107400	0.09602600
C	-4.33615400	-0.27933300	0.69535500
C	-5.23485200	0.77403000	0.74430500

C	-4.87354200	2.01884300	0.16678000
H	-3.37236200	3.10908700	-0.89004500
H	-4.58797200	-1.24396500	1.12711400
H	-5.56838300	2.85354900	0.19492300
O	-2.26390400	-1.21083200	0.11646000
C	-1.47273800	1.37037500	-1.19886600
H	-1.43589500	2.37741500	-1.63991800
N	-0.44211300	0.59952900	-1.39105300
C	0.61013900	1.12001400	-2.27034700
H	0.48393400	2.20419700	-2.40377000
H	0.47775100	0.66539700	-3.26181800
C	2.05902000	0.79007100	-1.88175100
H	2.69225700	1.27303300	-2.64730700
H	2.21497800	-0.28860300	-1.97180900
Zn	-0.39705600	-1.33650700	-0.47374200
C	3.97701900	0.91738600	-0.43015100
C	2.23118400	2.60925300	-0.22504500
H	1.76217300	0.12740600	0.51239300
C	4.53793700	1.26975400	0.95062500
H	4.51457700	1.49413200	-1.20526300
H	4.13179700	-0.14471700	-0.64396200
C	2.72920900	2.99992200	1.16974500
H	2.70071000	3.26103500	-0.98579400
H	1.15039700	2.75991500	-0.28216500
C	4.23031500	2.72588000	1.32313500
H	5.61823700	1.08398300	0.94873300
H	4.10636700	0.59335000	1.69980400
H	2.50604800	4.05958800	1.34029400
H	2.16565500	2.43145700	1.92105600
H	4.56057000	2.94103100	2.34597400
H	4.79373800	3.39881100	0.66106100
N	2.52280200	1.19194800	-0.53175300
Cl	0.86475900	-2.69131000	-1.92294400
C	1.52859500	-1.69586100	1.50850600
N	0.34484500	-2.56038700	1.37009300
H	0.60061700	-3.54230900	1.31264800
H	-0.28542500	-2.41756100	2.15647200
N	1.91612000	-1.51457300	2.88340700
H	2.45175600	-2.31868400	3.20074300
H	2.49456600	-0.68555100	2.98065400
O	2.58488200	-2.23597800	0.76029700
H	2.25274400	-2.47674300	-0.13472900
O	1.07095600	-0.46812100	0.97828000
C	-6.58504800	0.61498000	1.40182200
H	-7.39421600	0.84537900	0.69840700
H	-6.73529700	-0.40319400	1.77079100
H	-6.69155400	1.30287800	2.24965400

3a

C	-0.84038300	3.22310800	-0.86114500
C	-0.91729800	1.81223900	-0.73624200
C	-2.06854000	1.24616600	-0.09297700
C	-3.06793900	2.13753600	0.37520300
C	-2.97115500	3.51700400	0.24006400
C	-1.82916800	4.06444400	-0.38978700

H	0.03469900	3.64801500	-1.34853400
H	-3.94302600	1.69206200	0.84116800
H	-1.73460800	5.14040100	-0.50598600
O	-2.24132400	-0.04674000	0.09269200
C	0.18968900	1.06317800	-1.28800600
H	0.97996100	1.68495100	-1.72453600
N	0.34559600	-0.22310500	-1.34482200
C	1.57163000	-0.74939500	-1.94708700
H	2.01540900	-0.00663600	-2.62355700
H	1.30478400	-1.62691700	-2.54647200
C	2.59185700	-1.16942800	-0.87379900
H	3.36413600	-1.80205000	-1.35062300
H	2.07760700	-1.80148900	-0.14175700
Zn	-1.14084000	-1.52088200	-0.69011400
C	3.53170600	-0.32133400	1.21645800
C	4.31662300	0.54776800	-0.90450200
C	3.98159800	0.94579700	1.95206500
H	4.33875700	-1.08246300	1.27163100
H	2.65066700	-0.74809500	1.70763200
C	4.79989600	1.84744300	-0.25241200
H	5.15742000	-0.17688400	-0.94666300
H	4.01474200	0.73954900	-1.93993700
C	5.15272400	1.62000100	1.22396200
H	4.26152000	0.68764000	2.98076600
H	3.13236500	1.63886000	2.00832400
H	5.66670700	2.22957500	-0.80524600
H	4.00549900	2.60116400	-0.32962000
H	5.41442400	2.56801900	1.70884600
H	6.04152100	0.97573900	1.28997000
N	3.17969100	-0.02708500	-0.17722100
Cl	-1.68210500	-3.21641700	-2.06743400
C	-1.27124800	-2.28257900	2.26135600
N	-2.24824800	-1.40503600	2.49175400
H	-2.73092400	-1.40826000	3.37682900
H	-2.48062700	-0.74318500	1.73682600
O	-0.99535800	-3.08783900	3.30541300
H	-0.31286300	-3.71214300	3.01272700
O	-0.63344100	-2.38919300	1.19535400
C	-4.06521600	4.42640600	0.74618600
H	-4.48658500	5.02401600	-0.07092900
H	-4.87987600	3.85970400	1.20509000
H	-3.67767500	5.13061400	1.49216600

1b

C	3.99663800	1.75391200	-0.01745900
C	2.77589600	1.02261400	-0.06163200
C	2.83235300	-0.41840400	-0.12382900
C	4.12782000	-1.02049400	-0.14523700
C	5.29768100	-0.28420400	-0.09719400
C	5.22627500	1.13479900	-0.03079400
H	3.94398300	2.84059000	0.02628700
H	4.15314700	-2.10532200	-0.19474900
H	6.13914600	1.72288100	0.00531400
O	1.78754500	-1.17889400	-0.16791100

C	1.56852900	1.79237600	-0.07491300
H	1.73966300	2.87831000	-0.08415500
N	0.32469300	1.39231500	-0.08838400
C	-0.68825600	2.44355100	-0.19036500
H	-0.99581100	2.54251600	-1.24042000
H	-0.26080900	3.41499200	0.09869900
C	-1.91478000	2.19882900	0.69523200
H	-2.49015000	3.14344100	0.75911600
H	-1.57002800	1.94871300	1.70300400
Zn	-0.10846100	-0.68448000	0.08225000
C	-3.70843500	0.62952400	1.25293100
C	-3.45687200	1.37800400	-1.02283100
C	-4.15974900	-0.79678700	0.89201100
H	-4.57630100	1.30906300	1.35825500
H	-3.19581800	0.57930000	2.21494500
C	-4.47185200	0.25880100	-1.34378800
H	-4.00232300	2.34135900	-0.99233700
H	-2.71896500	1.43213800	-1.82548400
H	-5.19165000	-0.98962400	1.19925300
H	-3.48093800	-1.52636900	1.33826700
H	-5.48653100	0.51791500	-1.02998100
H	-4.48018400	0.02746300	-2.41050500
H	-3.07116200	-1.21874800	-0.90487700
H	-4.64551000	-1.77207400	-0.89319600
N	-2.76750300	1.09826900	0.23803600
Cl	-1.01661500	-1.35670800	2.11737400
Cl	-1.37649600	-1.53060100	-1.79029200
C	6.64629800	-0.96350700	-0.11369200
H	6.54781800	-2.05065100	-0.17464500
H	7.24490800	-0.62674200	-0.96900200
H	7.21739200	-0.72364300	0.79169900
N	-4.07330400	-0.97769800	-0.60261400

2b

C	-3.92462600	-1.89811100	-0.39742400
C	-2.78711700	-1.17093700	0.04782200
C	-2.87434600	0.26187300	0.13972400
C	-4.11804300	0.86603100	-0.21031700
C	-5.21174400	0.13461700	-0.64350400
C	-5.10684100	-1.27805100	-0.74116100
H	-3.85058900	-2.98251800	-0.45959100
H	-4.17326200	1.94784900	-0.12498400
H	-5.95786600	-1.86404700	-1.07697000
O	-1.88951400	1.01925500	0.51828500
C	-1.63561100	-1.94204700	0.42337500
H	-1.79505800	-3.02721700	0.34283700
N	-0.47039600	-1.54884300	0.85576700
C	0.42513300	-2.63693100	1.28610800
H	0.21448600	-3.53869600	0.69241700
H	0.19461100	-2.89260000	2.32972600
C	1.91684200	-2.29832400	1.24278400
H	2.47492800	-3.22501300	1.48929300
H	2.13644500	-1.57169100	2.02966000
Zn	0.00647700	0.54896500	0.89761900

C	3.70328300	-1.12100000	0.12202600
C	2.29109100	-2.55522100	-1.19192000
C	4.21679900	-0.63564000	-1.25255700
H	4.42557000	-1.85382300	0.53199700
H	3.63634000	-0.29168900	0.83171700
C	2.36102300	-1.66617800	-2.45676400
H	3.10334600	-3.30967700	-1.20107200
H	1.34919200	-3.10868000	-1.19612500
H	4.90182700	-1.37716800	-1.69273500
H	4.77089600	0.29981300	-1.13824500
H	2.86989000	-2.21457900	-3.26355500
H	1.35350700	-1.41286100	-2.80206900
H	1.89999600	0.57700400	-1.33753000
H	3.37136600	0.03940800	-3.00089600
N	2.36489400	-1.70580000	-0.01059500
Cl	1.53382500	0.96631900	2.63753400
C	1.41076100	2.45140300	-0.67986300
N	0.30314700	2.87524600	0.15430900
H	0.53272200	3.68670900	0.71772400
H	-0.54594800	3.02919100	-0.38302500
N	1.48235100	3.15208900	-1.94021900
H	1.75979500	4.11613600	-1.77010900
H	2.19596200	2.73259200	-2.53162900
O	2.61172500	2.60366500	0.03523700
H	2.49872300	2.17211900	0.91116000
O	1.12699000	1.07924300	-0.91307100
C	-6.50881300	0.81618800	-1.00957100
H	-7.33277400	0.45372100	-0.38288700
H	-6.44186700	1.90067500	-0.88761700
H	-6.78213400	0.60681700	-2.05099800
N	3.06003400	-0.39718600	-2.13630300

3b

C	-4.01468100	-1.50142900	-0.92592400
C	-2.72392300	-1.04679300	-0.54688100
C	-2.59389400	0.26665900	0.02972300
C	-3.78637500	1.02843600	0.18944000
C	-5.03763700	0.55755500	-0.17965500
C	-5.14821400	-0.73482800	-0.75195400
H	-4.10189500	-2.49359800	-1.36507300
H	-3.68196500	2.01180900	0.64075100
H	-6.12114500	-1.11696200	-1.04776000
O	-1.45121200	0.78626900	0.38791100
C	-1.62403300	-1.93932600	-0.79871800
H	-1.90669900	-2.86508600	-1.32063600
N	-0.37279700	-1.77564000	-0.49128800
C	0.57141500	-2.82222200	-0.90217200
H	0.63639400	-2.84363400	-1.99879800
H	0.21780100	-3.81353300	-0.58747600
C	1.95861700	-2.59636800	-0.28763500
H	2.66826900	-3.31559900	-0.73533500
H	1.91073300	-2.79320600	0.78757700
Zn	0.30162700	-0.19872700	0.75316600
C	3.65762200	-0.96099200	0.32566900

C	2.70260500	-0.85644600	-1.84582300
C	4.01077300	0.53206200	0.32962300
H	4.48467800	-1.56361200	-0.09763600
H	3.49222900	-1.27821500	1.35909500
C	2.95436600	0.64640400	-1.97203500
H	3.56964000	-1.43827400	-2.21529700
H	1.84456800	-1.10900600	-2.47524500
H	5.03813500	0.65847500	0.68593900
H	3.34931900	1.03208400	1.03543300
H	3.32874100	0.87513400	-2.97533700
H	1.98953200	1.14833600	-1.87200700
H	2.91216200	2.79649500	-0.63812600
H	4.82691900	1.26008100	-1.41460400
N	2.42404500	-1.20816100	-0.44545600
Cl	0.94372000	-0.96487700	2.82070800
C	1.10982700	2.72858100	-0.04602700
N	-0.09433500	3.31593200	-0.08602100
H	-0.22473800	4.17658800	-0.59420100
H	-0.88178500	2.71307600	0.16304000
O	2.12309300	3.41596200	-0.57600100
O	1.29937700	1.60407000	0.45332600
C	-6.27605900	1.39715200	0.02512600
H	-6.98891600	0.88804800	0.68491700
H	-6.03664100	2.36664500	0.47046900
H	-6.79125500	1.57668300	-0.92630400
N	3.90613600	1.21799600	-0.98992400