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Synthesis of amantadine-based novel Schiff base and its transition metal complexes as potential ALP, α-amylase, and α-glucosidase inhibitors

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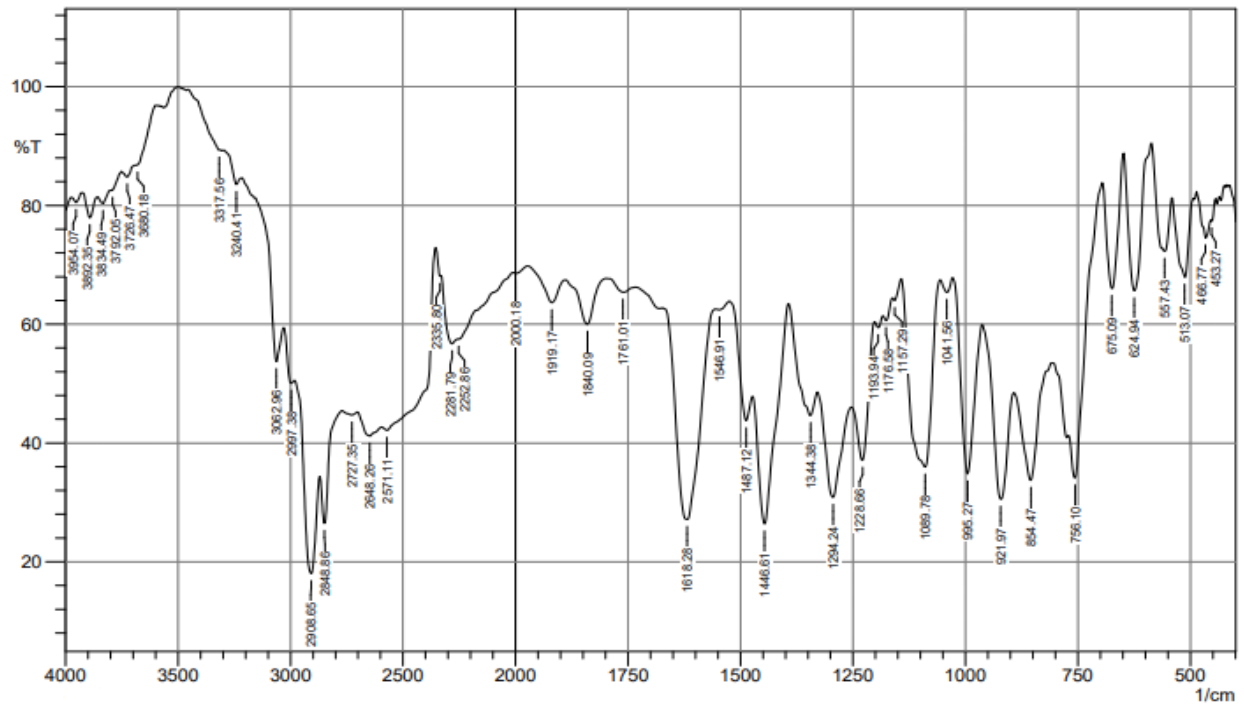

Figure S1. FT-IR spectrum of (E)-2-((adamantan-1-ylimino)methyl)-6-allylphenol (HL)

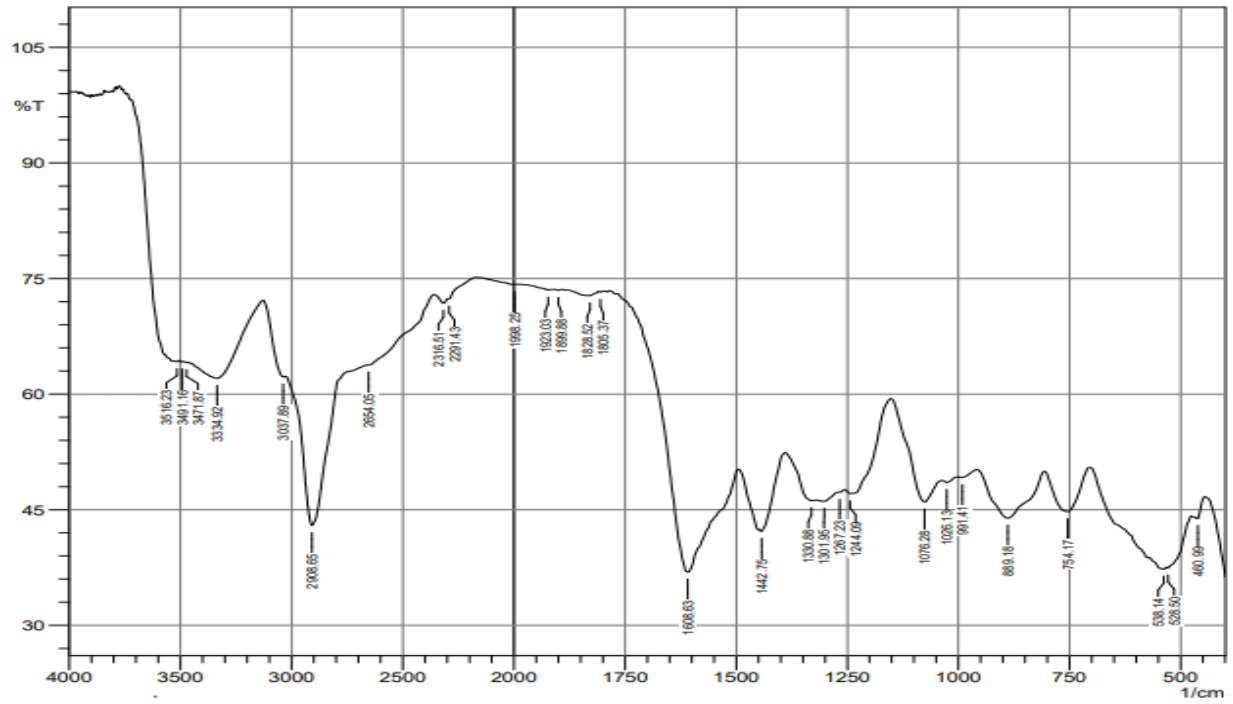

Figure S2. FT-IR spectrum of Cr(III) complex

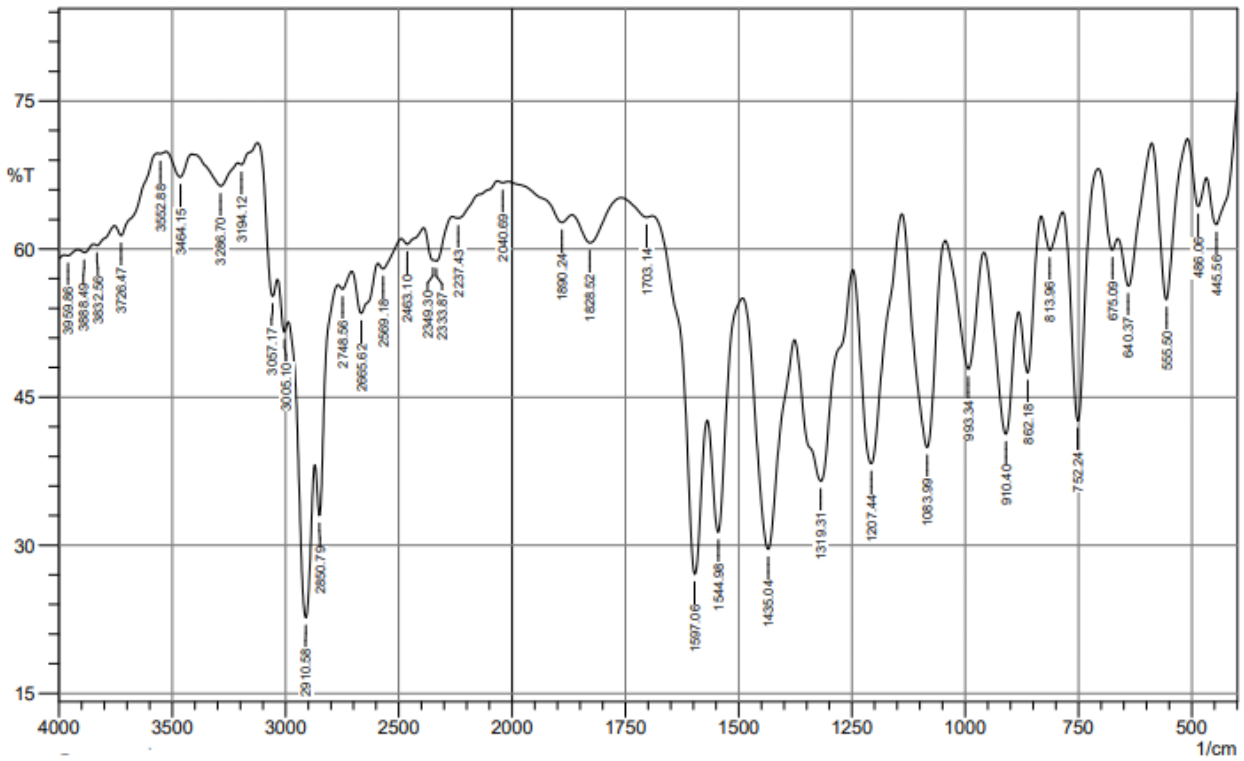

Figure S3. FT-IR spectrum of Co(II) complex

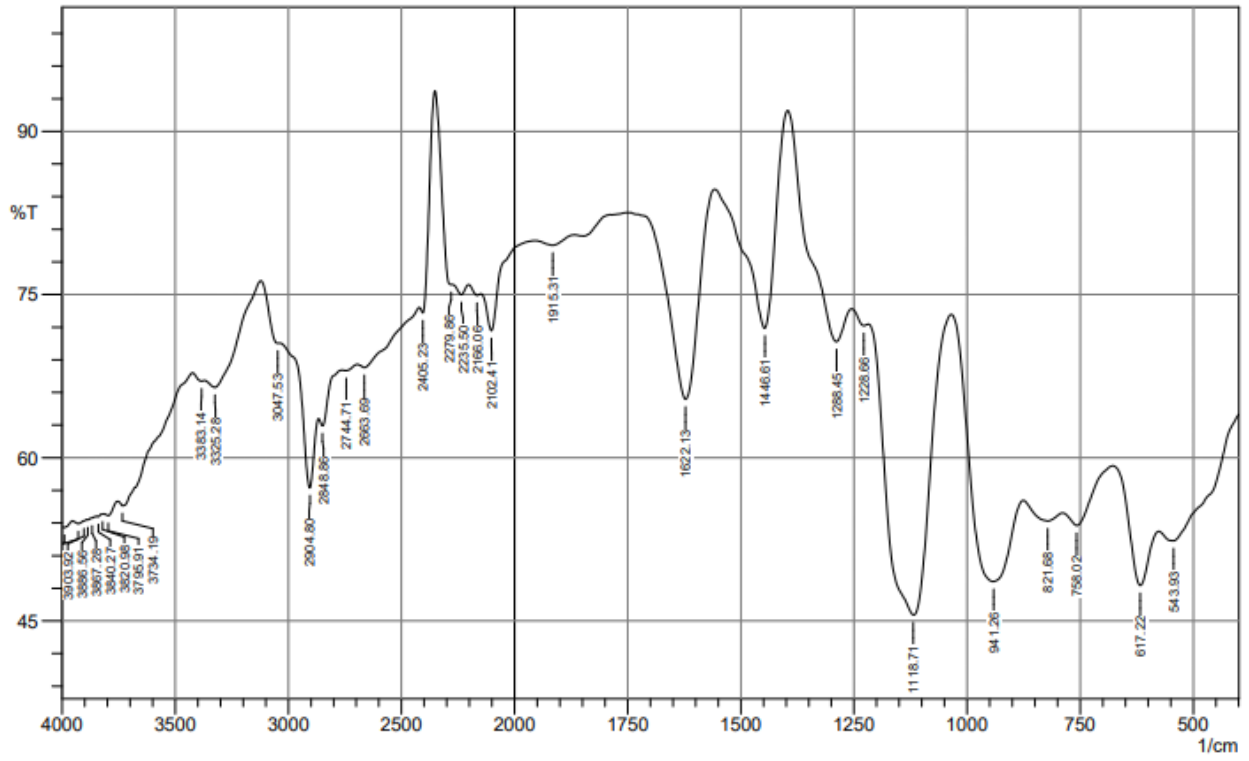

Figure S4. FT-IR spectrum of VO(IV) complex

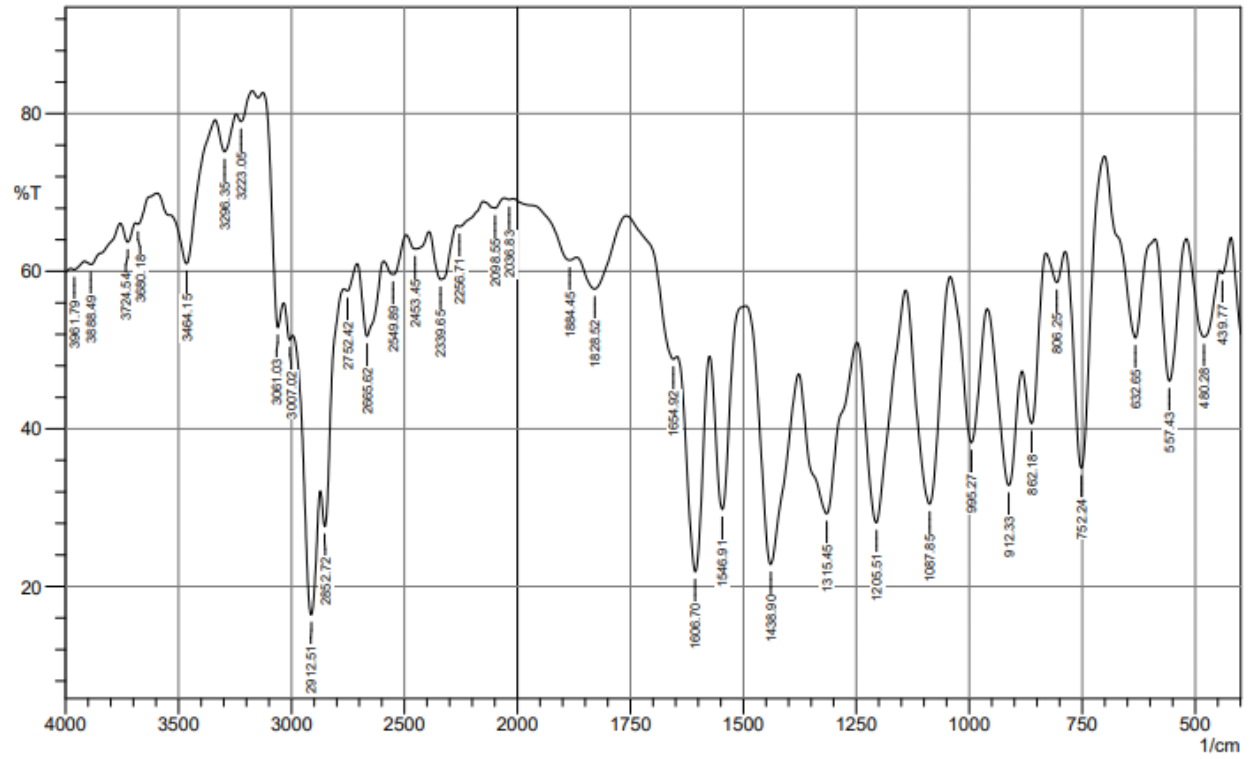

Figure S5. FT-IR spectrum of Zn(II) complex

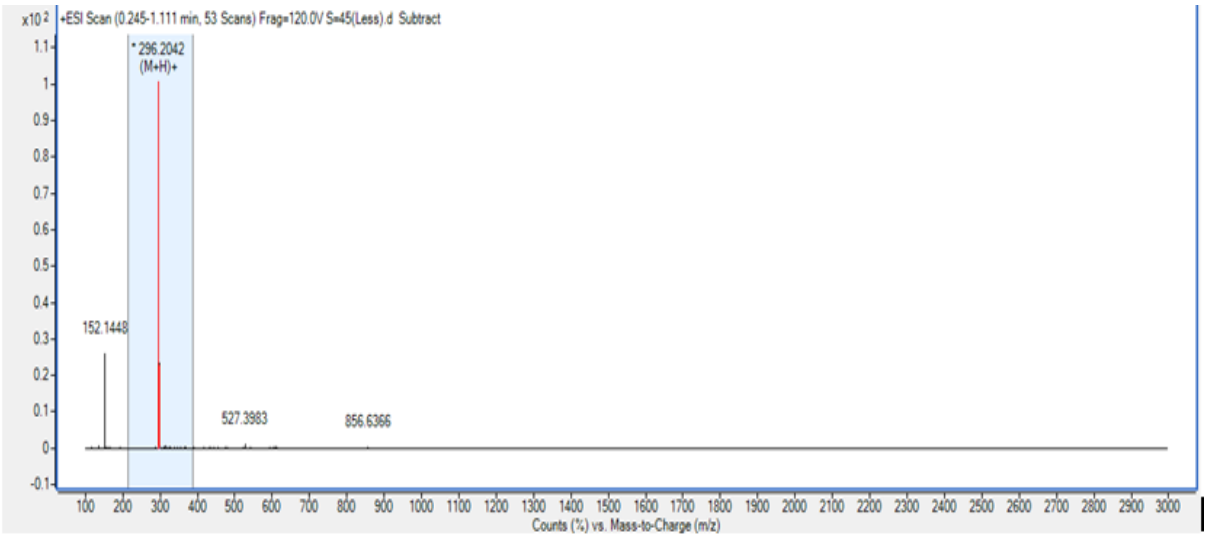

Figure S6. Mass spectrum of (E)-2-((adamantan-1-ylimino)methyl)-6-allylphenol

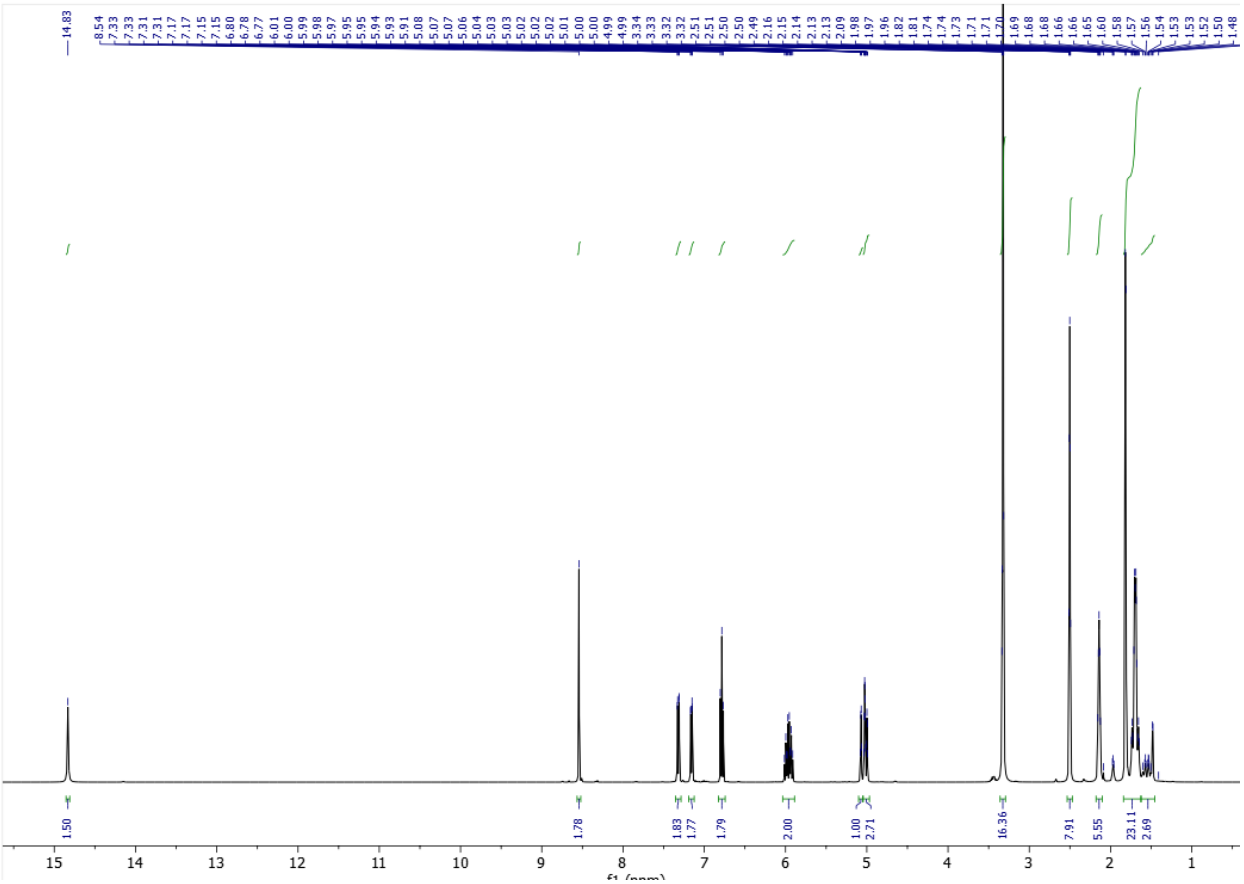

Figure S7. ^{1}H-NMR spectrum of (E)-2-((adamantan-1-ylimino)methyl)-6-allylphenol

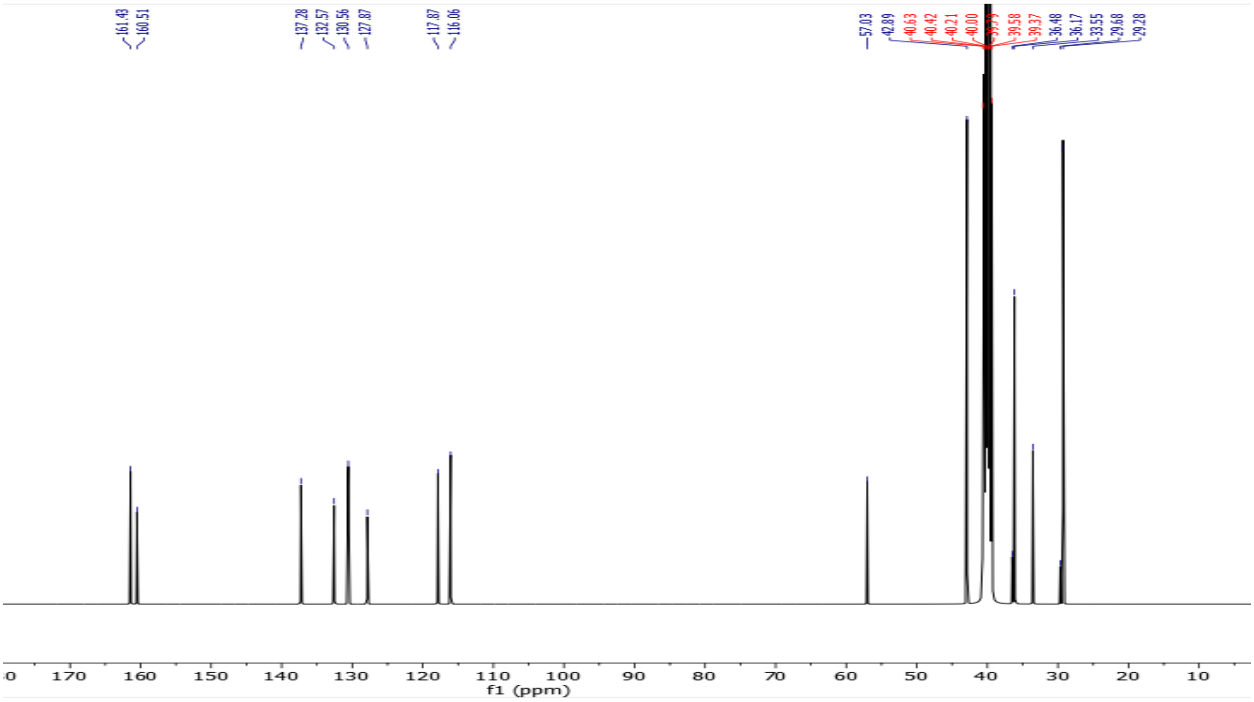

Figure S8. ^{13}C-NMR spectrum of (E)-2-((adamantan-1-ylimino)methyl)-6-allylphenol

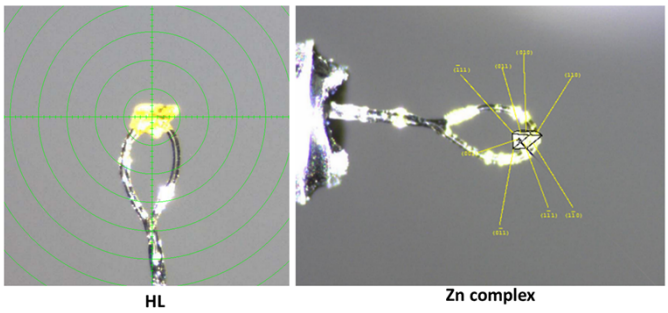

Figure S9. Single crystals of HL (left) and Zn complex (right) used for the collection of X-ray diffraction data

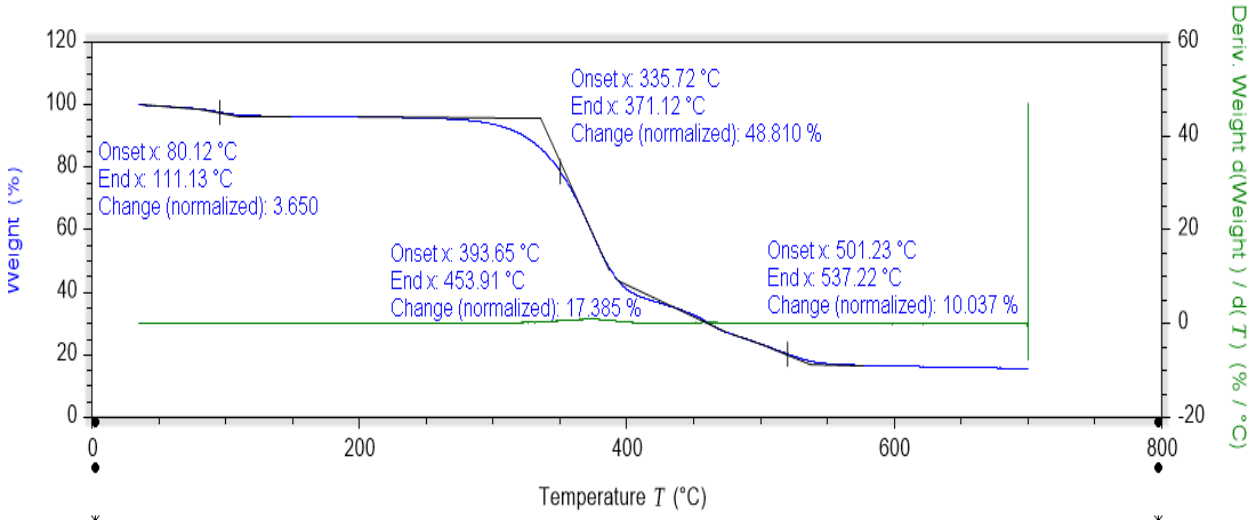

Figure S10. Thermogram of Zinc(II) complex

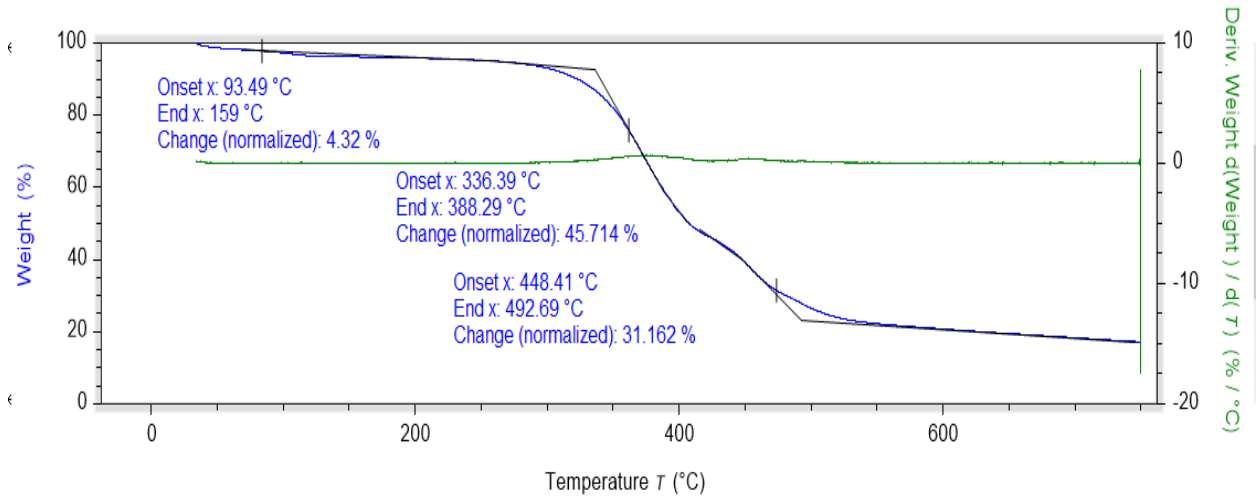

Figure S11. Thermogram of cobalt(II) complex

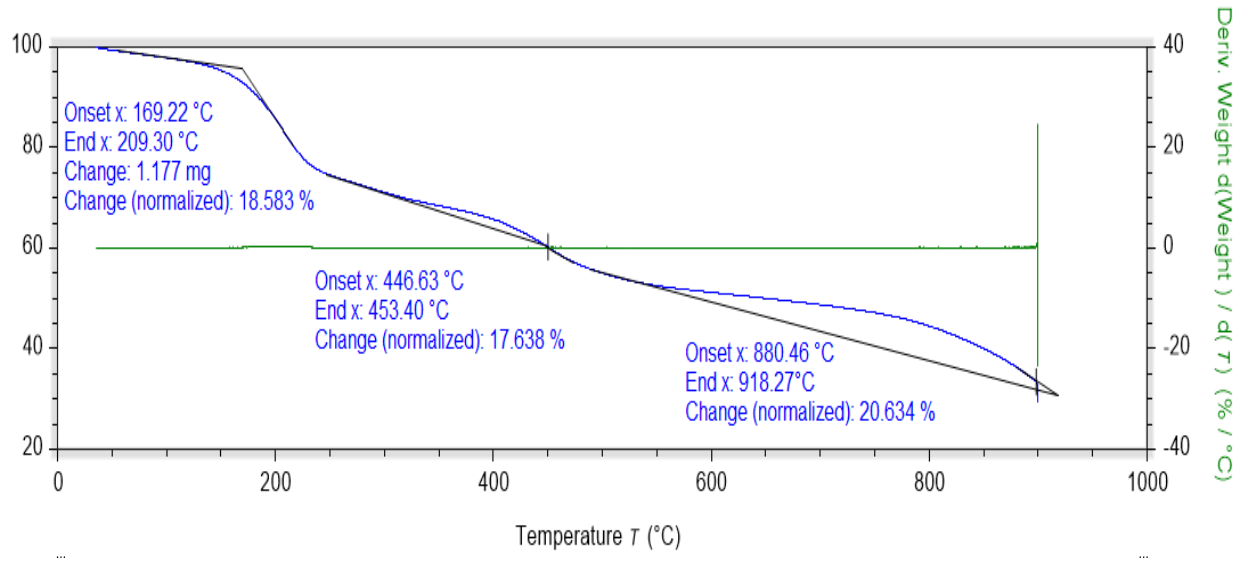

Figure S12. Thermogram of chromium(III) complex

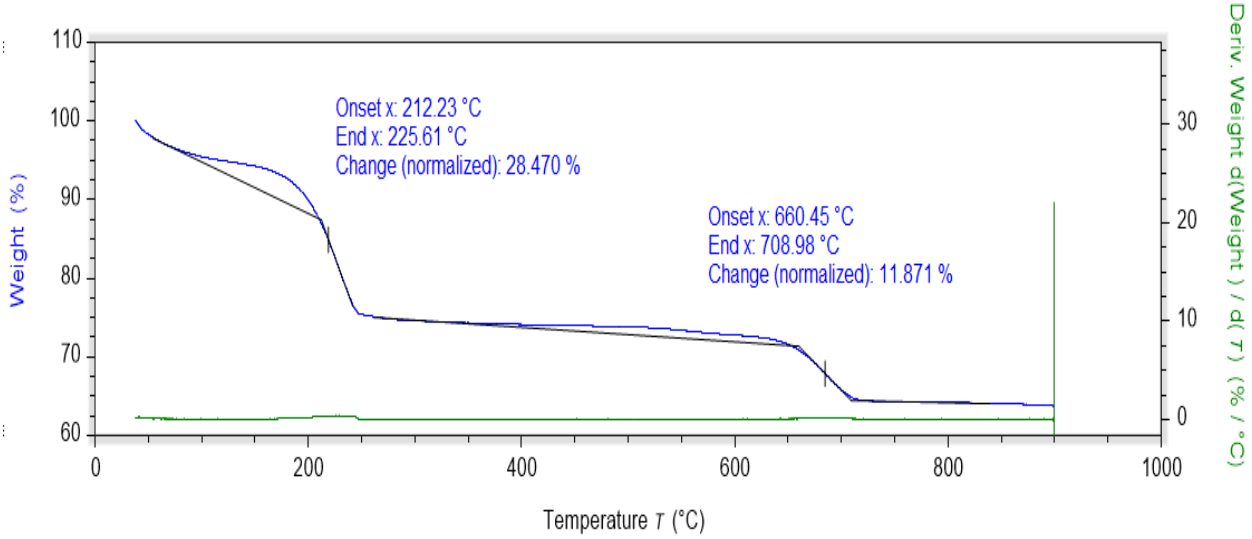

Figure S13. Thermogram of Oxovanadium(IV) complex

Table S1. Experimental details

Crystal data		
Chemical formula	$C_{20}H_{25}NO$	$C_{40}H_{48}N_2O_2Zn \cdot H_2O$
CCDC Number	2231982	2231983
M_r	295.41	672.19
Crystal system, space group	Monoclinic, *Pc*	Monoclinic, $P2_1/c$
Temperature (K)	100 (1)	
a, *b*, *c* (Å)	7.0706 (15), 18.748 (4), 12.612 (3)	23.960 (11), 10.415 (5), 13.692 (7)
θ (°)	105.578 (5)	95.301 (13)
V (Å^3)	1610.4 (6)	3402 (3)
Z	4	4
Radiation type	Microfocus Mo *K*α	
μ (mm^{-1})	0.07	0.76
Crystal size (mm)	0.25 × 0.19 × 0.15	0.15 × 0.09 × 0.06
Crystal Color	Yellow	Colorless
Data collection		
Diffractometer	Bruker D8 Venture PHOTON II detector (Bruker, 2016)	
Absorption correction	Multiscan (SADABS, Bruker 2016)	Analytical (SADABS, Bruker 2016)
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33731, 6004, 2414	68222, 6248, 3498
R_{int}	0.162	0.151
(sin θ/λ$_{max}$ (Å^{-1})	0.618	0.603
Refinement		
$R[F^2 > 2\ \sigma\ (F^2)]$, $wR(F^2)$, *S*	0.143, 0.435, 1.25	0.067, 0.238, 1.10
No. of reflections	6004	6248
No. of parameters	405	436
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	
Δp$_{max}$, Δp$_{min}$ (e Å^{-3})	0.72, -0.51	0.94, -0.93

Table S2. Bond distances and angles for Ligand (HL)

O1—C9	1.351 (16)	C3—H3A	0.9900
O2—C29	1.333 (15)	C3—H3B	0.9900
N1—C10	1.254 (16)	C3—C2	1.49 (2)
N1—C11	1.456 (16)	C19—H19A	0.9900
N2—C30	1.275 (17)	C19—H19B	0.9900
N2—C31	1.483 (17)	C34—H34A	0.9900
C29—C28	1.414 (18)	C34—H34B	0.9900
C29—C24	1.429 (18)	C34—C38	1.53 (2)
C4—C9	1.401 (17)	C34—C32	1.517 (19)

C4—C5	1.389 (19)	C26—H26	0.9500
C4—C3	1.521 (19)	C26—C27	1.356 (19)
C9—C8	1.39 (2)	C2—H2	0.9500
C8—C10	1.468 (19)	C2—C1	1.27 (2)
C8—C7	1.40 (2)	C37—H37A	0.9900
C20—H20A	0.9900	C37—H37B	0.9900
C20—H20B	0.9900	C37—C38	1.534 (19)
C20—C18	1.507 (17)	C37—C36	1.50 (2)
C20—C11	1.520 (19)	C27—H27	0.9500
C15—H15A	0.9900	C33—H33A	0.9900
C15—H15B	0.9900	C33—H33B	0.9900
C15—C13	1.50 (2)	C33—C32	1.49 (2)
C15—C18	1.53 (2)	C33—C36	1.52 (2)
C10—H10	0.9500	C30—H30	0.9500
C28—C27	1.37 (2)	C31—C35	1.51 (2)
C28—C30	1.470 (18)	C31—C39	1.520 (19)
C13—H13	1.0000	C31—C40	1.529 (18)
C13—C12	1.489 (18)	C14—H14A	0.9900
C13—C14	1.519 (19)	C14—H14B	0.9900
C17—H17A	0.9900	C35—H35A	0.9900
C17—H17B	0.9900	C35—H35B	0.9900
C17—C18	1.53 (2)	C35—C36	1.54 (2)
C17—C16	1.52 (2)	C23—H23A	0.9900
C6—H6	0.9500	C23—H23B	0.9900
C6—C5	1.39 (2)	C23—C22	1.48 (2)
C6—C7	1.418 (19)	C38—H38	1.0000
C18—H18	1.0000	C38—C39	1.507 (18)
C24—C25	1.353 (19)	C39—H39A	0.9900
C24—C23	1.537 (19)	C39—H39B	0.9900
C5—H5	0.9500	C32—H32	1.0000
C16—H16	1.0000	C32—C40	1.48 (2)
C16—C19	1.529 (19)	C40—H40A	0.9900
C16—C14	1.54 (2)	C40—H40B	0.9900
C25—H25	0.9500	C36—H36	1.0000
C25—C26	1.43 (2)	C22—H22	0.9500
C12—H12A	0.9900	C22—C21	1.28 (2)
C12—H12B	0.9900	C1—H1A	0.9500
C12—C11	1.566 (19)	C1—H1B	0.9500

C7—H7	0.9500	C21—H21A	0.9500
C11—C19	1.517 (19)	C21—H21B	0.9500
Bond angles			
C10—N1—C11	122.4 (12)	H19A—C19—H19B	107.9
C30—N2—C31	121.3 (11)	H34A—C34—H34B	108.2
O2—C29—C28	123.6 (12)	C38—C34—H34A	109.8
O2—C29—C24	118.1 (11)	C38—C34—H34B	109.8
C28—C29—C24	118.4 (12)	C32—C34—H34A	109.8
C9—C4—C3	120.2 (12)	C32—C34—H34B	109.8
C5—C4—C9	117.9 (13)	C32—C34—C38	109.5 (11)
C5—C4—C3	121.8 (12)	C25—C26—H26	120.8
O1—C9—C4	118.3 (12)	C27—C26—C25	118.4 (14)
O1—C9—C8	121.1 (12)	C27—C26—H26	120.8
C8—C9—C4	120.5 (13)	C3—C2—H2	115.7
C9—C8—C10	121.7 (12)	C1—C2—C3	128.7 (19)
C9—C8—C7	121.0 (13)	C1—C2—H2	115.7
C7—C8—C10	117.3 (14)	H37A—C37—H37B	108.3
H20A—C20—H20B	108.1	C38—C37—H37A	109.8
C18—C20—H20A	109.5	C38—C37—H37B	109.8
C18—C20—H20B	109.5	C36—C37—H37A	109.8
C18—C20—C11	110.5 (11)	C36—C37—H37B	109.8
C11—C20—H20A	109.5	C36—C37—C38	109.2 (12)
C11—C20—H20B	109.5	C28—C27—H27	119.0
H15A—C15—H15B	108.3	C26—C27—C28	122.0 (14)
C13—C15—H15A	109.9	C26—C27—H27	119.0
C13—C15—H15B	109.9	H33A—C33—H33B	108.1
C13—C15—C18	108.8 (12)	C32—C33—H33A	109.5
C18—C15—H15A	109.9	C32—C33—H33B	109.5
C18—C15—H15B	109.9	C32—C33—C36	110.7 (13)
N1—C10—C8	121.7 (13)	C36—C33—H33A	109.5
N1—C10—H10	119.1	C36—C33—H33B	109.5
C8—C10—H10	119.1	N2—C30—C28	122.5 (13)
C29—C28—C30	119.7 (13)	N2—C30—H30	118.7
C27—C28—C29	120.2 (12)	C28—C30—H30	118.7
C27—C28—C30	120.1 (13)	N2—C31—C35	106.4 (11)
C15—C13—H13	108.7	N2—C31—C39	108.3 (10)
C15—C13—C14	110.3 (12)	N2—C31—C40	114.9 (11)
C12—C13—C15	110.2 (12)	C35—C31—C39	109.0 (11)

C12—C13—H13	108.7	C35—C31—C40	107.9 (12)
C12—C13—C14	110.3 (12)	C39—C31—C40	110.1 (11)
C14—C13—H13	108.7	C13—C14—C16	109.3 (13)
H17A—C17—H17B	108.2	C13—C14—H14A	109.8
C18—C17—H17A	109.7	C13—C14—H14B	109.8
C18—C17—H17B	109.7	C16—C14—H14A	109.8
C16—C17—H17A	109.7	C16—C14—H14B	109.8
C16—C17—H17B	109.7	H14A—C14—H14B	108.3
C16—C17—C18	109.8 (13)	C31—C35—H35A	109.6
C5—C6—H6	120.8	C31—C35—H35B	109.6
C5—C6—C7	118.5 (13)	C31—C35—C36	110.3 (13)
C7—C6—H6	120.8	H35A—C35—H35B	108.1
C20—C18—C15	109.5 (12)	C36—C35—H35A	109.6
C20—C18—C17	110.2 (12)	C36—C35—H35B	109.6
C20—C18—H18	109.3	C24—C23—H23A	109.0
C15—C18—H18	109.3	C24—C23—H23B	109.0
C17—C18—C15	109.2 (12)	H23A—C23—H23B	107.8
C17—C18—H18	109.3	C22—C23—C24	112.9 (13)
C29—C24—C23	119.6 (12)	C22—C23—H23A	109.0
C25—C24—C29	119.3 (12)	C22—C23—H23B	109.0
C25—C24—C23	121.0 (13)	C34—C38—C37	109.5 (12)
C4—C5—H5	118.5	C34—C38—H38	109.3
C6—C5—C4	122.9 (13)	C37—C38—H38	109.3
C6—C5—H5	118.5	C39—C38—C34	109.5 (12)
C17—C16—H16	110.3	C39—C38—C37	109.8 (12)
C17—C16—C19	108.5 (13)	C39—C38—H38	109.3
C17—C16—C14	108.5 (13)	C31—C39—H39A	109.9
C19—C16—H16	110.3	C31—C39—H39B	109.9
C19—C16—C14	108.9 (12)	C38—C39—C31	109.0 (11)
C14—C16—H16	110.3	C38—C39—H39A	109.9
C24—C25—H25	119.1	C38—C39—H39B	109.9
C24—C25—C26	121.7 (14)	H39A—C39—H39B	108.3
C26—C25—H25	119.1	C34—C32—H32	109.5
C13—C12—H12A	109.6	C33—C32—C34	108.9 (12)
C13—C12—H12B	109.6	C33—C32—H32	109.5
C13—C12—C11	110.3 (11)	C40—C32—C34	109.4 (12)
H12A—C12—H12B	108.1	C40—C32—C33	110.2 (13)
C11—C12—H12A	109.6	C40—C32—H32	109.5

C11—C12—H12B	109.6	C31—C40—H40A	109.5
C8—C7—C6	118.9 (14)	C31—C40—H40B	109.5
C8—C7—H7	120.5	C32—C40—C31	110.6 (12)
C6—C7—H7	120.5	C32—C40—H40A	109.5
N1—C11—C20	109.9 (10)	C32—C40—H40B	109.5
N1—C11—C12	115.3 (10)	H40A—C40—H40B	108.1
N1—C11—C19	107.4 (11)	C37—C36—C33	109.8 (12)
C20—C11—C12	107.5 (11)	C37—C36—C35	108.0 (12)
C19—C11—C20	109.0 (11)	C37—C36—H36	110.0
C19—C11—C12	107.5 (11)	C33—C36—C35	109.1 (13)
C4—C3—H3A	108.8	C33—C36—H36	110.0
C4—C3—H3B	108.8	C35—C36—H36	110.0
H3A—C3—H3B	107.7	C23—C22—H22	115.5
C2—C3—C4	113.7 (12)	C21—C22—C23	128.9 (18)
C2—C3—H3A	108.8	C21—C22—H22	115.5
C2—C3—H3B	108.8	C2—C1—H1A	120.0
C16—C19—H19A	109.2	C2—C1—H1B	120.0
C16—C19—H19B	109.2	H1A—C1—H1B	120.0
C11—C19—C16	111.9 (12)	C22—C21—H21A	120.0
C11—C19—H19A	109.2	C22—C21—H21B	120.0
C11—C19—H19B	109.2	H21A—C21—H21B	120.0
Torsions			
O1—C9—C8—C10	5 (2)	C5—C4—C3—C2	25 (2)
O1—C9—C8—C7	-176.2 (13)	C5—C6—C7—C8	-4 (2)
O2—C29—C28—C27	178.5 (14)	C16—C17—C18—C20	-59.9 (17)
O2—C29—C28—C30	-5.1 (19)	C16—C17—C18—C15	60.5 (16)
O2—C29—C24—C25	-178.2 (12)	C25—C24—C23—C22	-28 (2)
O2—C29—C24—C23	-0.5 (19)	C25—C26—C27—C28	2 (2)
N1—C11—C19—C16	177.1 (11)	C12—C13—C14—C16	60.8 (16)
N2—C31—C35—C36	-177.1 (11)	C12—C11—C19—C16	-58.2 (15)
N2—C31—C39—C38	175.2 (10)	C7—C8—C10—N1	179.8 (14)
N2—C31—C40—C32	-178.8 (11)	C7—C6—C5—C4	7 (2)
C29—C28—C27—C26	0 (2)	C11—N1—C10—C8	178.4 (12)
C29—C28—C30—N2	4.2 (19)	C11—C20—C18—C15	-60.8 (15)
C29—C24—C25—C26	0 (2)	C11—C20—C18—C17	59.3 (16)
C29—C24—C23—C22	154.5 (14)	C3—C4—C9—O1	-4.0 (19)
C4—C9—C8—C10	-177.0 (13)	C3—C4—C9—C8	177.9 (13)

C4—C9—C8—C7	2 (2)	C3—C4—C5—C6	177.7 (14)
C4—C3—C2—C1	-117 (2)	C19—C16—C14—C13	-58.4 (16)
C9—C4—C5—C6	-5 (2)	C34—C38—C39—C31	59.8 (14)
C9—C4—C3—C2	-152.1 (13)	C34—C32—C40—C31	-59.0 (15)
C9—C8—C10—N1	-1 (2)	C37—C38—C39—C31	-60.4 (15)
C9—C8—C7—C6	0 (2)	C27—C28—C30—N2	-179.4 (14)
C20—C11—C19—C16	58.0 (15)	C33—C32—C40—C31	60.7 (16)
C15—C13—C12—C11	60.8 (14)	C30—N2—C31—C35	-122.3 (14)
C15—C13—C14—C16	-61.1 (15)	C30—N2—C31—C39	120.6 (13)
C10—N1—C11—C20	-112.0 (14)	C30—N2—C31—C40	-3.0 (18)
C10—N1—C11—C12	9.7 (18)	C30—C28—C27—C26	-176.9 (14)
C10—N1—C11—C19	129.5 (14)	C31—N2—C30—C28	179.8 (12)
C10—C8—C7—C6	178.5 (13)	C31—C35—C36—C37	61.0 (16)
C28—C29—C24—C25	2 (2)	C31—C35—C36—C33	-58.4 (16)
C28—C29—C24—C23	179.5 (12)	C14—C13—C12—C11	-61.2 (16)
C13—C15—C18—C20	60.5 (15)	C14—C16—C19—C11	59.3 (16)
C13—C15—C18—C17	-60.3 (15)	C35—C31—C39—C38	59.9 (14)
C13—C12—C11—N1	178.6 (11)	C35—C31—C40—C32	-60.4 (16)
C13—C12—C11—C20	-58.4 (14)	C23—C24—C25—C26	-177.8 (14)
C13—C12—C11—C19	58.8 (15)	C38—C34—C32—C33	-60.2 (16)
C17—C16—C19—C11	-58.7 (16)	C38—C34—C32—C40	60.3 (15)
C17—C16—C14—C13	59.6 (16)	C38—C37—C36—C33	58.6 (16)
C18—C20—C11—N1	-175.2 (11)	C38—C37—C36—C35	-60.3 (15)
C18—C20—C11—C12	58.5 (13)	C39—C31—C35—C36	-60.5 (15)
C18—C20—C11—C19	-57.7 (14)	C39—C31—C40—C32	58.5 (15)
C18—C15—C13—C12	-60.9 (14)	C32—C34—C38—C37	59.4 (16)
C18—C15—C13—C14	61.1 (15)	C32—C34—C38—C39	-61.1 (15)
C18—C17—C16—C19	58.3 (16)	C32—C33—C36—C37	-60.7 (16)
C18—C17—C16—C14	-59.8 (16)	C32—C33—C36—C35	57.5 (16)
C24—C29—C28—C27	-2 (2)	C40—C31—C35—C36	59.1 (16)
C24—C29—C28—C30	174.9 (12)	C40—C31—C39—C38	-58.3 (14)
C24—C25—C26—C27	-2 (2)	C36—C37—C38—C34	-58.6 (15)
C24—C23—C22—C21	118.6 (19)	C36—C37—C38—C39	61.6 (16)
C5—C4—C9—O1	179.0 (12)	C36—C33—C32—C34	60.7 (16)
C5—C4—C9—C8	1 (2)	C36—C33—C32—C40	-59.3 (16)

Table S3. Bond distances and angles for Zn-Complex

Bond Lengths			
Zn1—O2	1.925 (4)	C12—H12B	0.9900
Zn1—O1	1.917 (4)	C12—C13	1.546 (9)
Zn1—N1	1.994 (5)	C32—H32A	0.9900
Zn1—N2	2.000 (5)	C32—H32B	0.9900
O2—C29	1.300 (7)	C32—C33	1.546 (9)
O1—C9	1.307 (7)	C6—H6	0.9500
N1—C31	1.490 (7)	C33—H33	1.0000
N1—C30	1.294 (7)	C33—C34	1.539 (8)
N2—C10	1.287 (7)	C33—C39	1.527 (9)
N2—C11	1.501 (8)	C34—H34A	0.9900
C8—C10	1.482 (8)	C34—H34B	0.9900
C8—C7	1.421 (8)	C40—H40A	0.9900
C8—C9	1.406 (8)	C40—H40B	0.9900
C31—C36	1.537 (8)	C40—C38	1.513 (9)
C31—C37	1.515 (8)	C25—H25	0.9500
C31—C32	1.540 (8)	C25—C26	1.406 (10)
C30—H30	0.9500	C2—H2	0.9500
C30—C28	1.469 (8)	C2—C1	1.311 (10)
C10—H10	0.9500	C38—H38	1.0000
C28—C29	1.420 (9)	C38—C39	1.532 (10)
C28—C27	1.415 (8)	C39—H39A	0.9900
C29—C24	1.422 (9)	C39—H39B	0.9900
C4—C9	1.425 (9)	C19—H19A	0.9900
C4—C5	1.383 (9)	C19—H19B	0.9900
C4—C3	1.509 (9)	C19—C18	1.531 (10)
C7—H7	0.9500	C19—C13	1.532 (9)
C7—C6	1.346 (9)	C23—H23	0.9500
C11—C20	1.526 (8)	C23—C22	1.422 (13)
C11—C12	1.523 (9)	C26—H26	0.9500
C11—C16	1.529 (9)	C18—H18	1.0000
C35—H35	1.0000	C18—C17	1.538 (10)
C35—C36	1.523 (9)	O3—H3C	0.8702
C35—C34	1.522 (9)	O3—H3D	0.8698
C35—C40	1.549 (9)	C1—H1A	0.96 (9)
C5—H5	0.9500	C1—H1B	1.11 (8)
C5—C6	1.390 (9)	C16—H16A	0.9900

C20—H20A	0.9900	C16—H16B	0.9900
C20—H20B	0.9900	C16—C15	1.540 (10)
C20—C18	1.542 (9)	C13—H13	1.0000
C36—H36A	0.9900	C13—C14	1.508 (11)
C36—H36B	0.9900	C15—H15	1.0000
C3—H3A	0.9900	C15—C17	1.543 (12)
C3—H3B	0.9900	C15—C14	1.528 (12)
C3—C2	1.514 (9)	C17—H17A	0.9900
C37—H37A	0.9900	C17—H17B	0.9900
C37—H37B	0.9900	C14—H14A	0.9900
C37—C38	1.545 (9)	C14—H14B	0.9900
C27—H27	0.9500	C21—H21A	0.9500
C27—C26	1.372 (9)	C21—H21B	0.9500
C24—C25	1.375 (9)	C21—C22	1.196 (13)
C24—C23	1.515 (9)	C22—H22	0.9500
C12—H12A	0.9900		
Bond angles			
O2—Zn1—N1	97.22 (19)	C33—C32—H32A	109.7
O2—Zn1—N2	111.1 (2)	C33—C32—H32B	109.7
O1—Zn1—O2	114.47 (18)	C7—C6—C5	119.4 (6)
O1—Zn1—N1	114.24 (19)	C7—C6—H6	120.3
O1—Zn1—N2	97.48 (18)	C5—C6—H6	120.3
N1—Zn1—N2	123.3 (2)	C32—C33—H33	109.6
C29—O2—Zn1	125.4 (4)	C34—C33—C32	109.0 (5)
C9—O1—Zn1	121.9 (4)	C34—C33—H33	109.6
C31—N1—Zn1	120.6 (4)	C39—C33—C32	108.5 (5)
C30—N1—Zn1	120.0 (4)	C39—C33—H33	109.6
C30—N1—C31	119.4 (5)	C39—C33—C34	110.5 (5)
C10—N2—Zn1	119.3 (4)	C35—C34—C33	109.8 (5)
C10—N2—C11	119.6 (5)	C35—C34—H34A	109.7
C11—N2—Zn1	120.9 (4)	C35—C34—H34B	109.7
C7—C8—C10	114.5 (5)	C33—C34—H34A	109.7
C9—C8—C10	125.8 (5)	C33—C34—H34B	109.7
C9—C8—C7	119.7 (5)	H34A—C34—H34B	108.2
N1—C31—C36	107.2 (5)	C35—C40—H40A	109.7
N1—C31—C37	115.5 (5)	C35—C40—H40B	109.7
N1—C31—C32	107.0 (4)	H40A—C40—H40B	108.2
C36—C31—C32	108.6 (5)	C38—C40—C35	109.8 (5)

C37—C31—C36	109.3 (5)	C38—C40—H40A	109.7
C37—C31—C32	109.0 (5)	C38—C40—H40B	109.7
N1—C30—H30	116.6	C24—C25—H25	119.5
N1—C30—C28	126.7 (6)	C24—C25—C26	120.9 (6)
C28—C30—H30	116.6	C26—C25—H25	119.5
N2—C10—C8	125.9 (5)	C3—C2—H2	118.0
N2—C10—H10	117.0	C1—C2—C3	124.1 (7)
C8—C10—H10	117.0	C1—C2—H2	118.0
C29—C28—C30	126.4 (5)	C37—C38—H38	109.3
C27—C28—C30	115.2 (6)	C40—C38—C37	110.2 (6)
C27—C28—C29	118.4 (6)	C40—C38—H38	109.3
O2—C29—C28	122.7 (6)	C40—C38—C39	109.8 (5)
O2—C29—C24	118.6 (6)	C39—C38—C37	108.8 (6)
C28—C29—C24	118.7 (6)	C39—C38—H38	109.3
C9—C4—C3	119.1 (6)	C33—C39—C38	109.5 (5)
C5—C4—C9	119.6 (6)	C33—C39—H39A	109.8
C5—C4—C3	121.3 (6)	C33—C39—H39B	109.8
C8—C7—H7	119.3	C38—C39—H39A	109.8
C6—C7—C8	121.4 (6)	C38—C39—H39B	109.8
C6—C7—H7	119.3	H39A—C39—H39B	108.2
N2—C11—C20	107.8 (5)	H19A—C19—H19B	108.3
N2—C11—C12	114.7 (5)	C18—C19—H19A	109.9
N2—C11—C16	105.6 (5)	C18—C19—H19B	109.9
C20—C11—C16	109.5 (6)	C18—C19—C13	109.1 (6)
C12—C11—C20	109.2 (5)	C13—C19—H19A	109.9
C12—C11—C16	109.9 (6)	C13—C19—H19B	109.9
C36—C35—H35	109.9	C24—C23—H23	121.3
C36—C35—C40	108.7 (5)	C22—C23—C24	117.4 (7)
C34—C35—H35	109.9	C22—C23—H23	121.3
C34—C35—C36	109.2 (5)	C27—C26—C25	118.9 (6)
C34—C35—C40	109.2 (5)	C27—C26—H26	120.5
C40—C35—H35	109.9	C25—C26—H26	120.5
O1—C9—C8	124.3 (5)	C20—C18—H18	109.7
O1—C9—C4	117.6 (5)	C19—C18—C20	108.8 (5)
C8—C9—C4	118.1 (5)	C19—C18—H18	109.7
C4—C5—H5	119.1	C19—C18—C17	109.7 (6)
C4—C5—C6	121.8 (6)	C17—C18—C20	109.3 (5)
C6—C5—H5	119.1	C17—C18—H18	109.7

C11—C20—H20A	109.7	H3C—O3—H3D	104.5
C11—C20—H20B	109.7	C2—C1—H1A	121 (5)
C11—C20—C18	109.9 (5)	C2—C1—H1B	126 (4)
H20A—C20—H20B	108.2	H1A—C1—H1B	110 (6)
C18—C20—H20A	109.7	C11—C16—H16A	109.7
C18—C20—H20B	109.7	C11—C16—H16B	109.7
C31—C36—H36A	109.4	C11—C16—C15	109.8 (6)
C31—C36—H36B	109.4	H16A—C16—H16B	108.2
C35—C36—C31	111.0 (5)	C15—C16—H16A	109.7
C35—C36—H36A	109.4	C15—C16—H16B	109.7
C35—C36—H36B	109.4	C12—C13—H13	109.1
H36A—C36—H36B	108.0	C19—C13—C12	109.7 (5)
C4—C3—H3A	109.1	C19—C13—H13	109.1
C4—C3—H3B	109.1	C14—C13—C12	110.0 (6)
C4—C3—C2	112.5 (5)	C14—C13—C19	110.0 (7)
H3A—C3—H3B	107.8	C14—C13—H13	109.1
C2—C3—H3A	109.1	C16—C15—H15	109.7
C2—C3—H3B	109.1	C16—C15—C17	108.0 (6)
C31—C37—H37A	109.7	C17—C15—H15	109.7
C31—C37—H37B	109.7	C14—C15—C16	109.9 (7)
C31—C37—C38	109.8 (5)	C14—C15—H15	109.7
H37A—C37—H37B	108.2	C14—C15—C17	109.6 (6)
C38—C37—H37A	109.7	C18—C17—C15	109.4 (6)
C38—C37—H37B	109.7	C18—C17—H17A	109.8
C28—C27—H27	118.9	C18—C17—H17B	109.8
C26—C27—C28	122.2 (6)	C15—C17—H17A	109.8
C26—C27—H27	118.9	C15—C17—H17B	109.8
C29—C24—C23	117.9 (6)	H17A—C17—H17B	108.2
C25—C24—C29	120.7 (6)	C13—C14—C15	109.8 (6)
C25—C24—C23	121.4 (6)	C13—C14—H14A	109.7
C11—C12—H12A	109.9	C13—C14—H14B	109.7
C11—C12—H12B	109.9	C15—C14—H14A	109.7
C11—C12—C13	108.9 (6)	C15—C14—H14B	109.7
H12A—C12—H12B	108.3	H14A—C14—H14B	108.2
C13—C12—H12A	109.9	H21A—C21—H21B	120.0
C13—C12—H12B	109.9	C22—C21—H21A	120.0
C31—C32—H32A	109.7	C22—C21—H21B	120.0
C31—C32—H32B	109.7	C23—C22—H22	107.8

C31—C32—C33	109.8 (5)	C21—C22—C23	144.4 (17)
H32A—C32—H32B	108.2	C21—C22—H22	107.8
Torsion angles			
Zn1—O2—C29—C28	-12.8 (8)	C11—C16—C15—C17	-61.5 (9)
Zn1—O2—C29—C24	166.8 (4)	C11—C16—C15—C14	58.1 (8)
Zn1—O1—C9—C8	-20.0 (8)	C35—C40—C38—C37	-59.4 (7)
Zn1—O1—C9—C4	159.3 (4)	C35—C40—C38—C39	60.5 (7)
Zn1—N1—C31—C36	42.7 (6)	C9—C8—C10—N2	10.0 (10)
Zn1—N1—C31—C37	164.8 (4)	C9—C8—C7—C6	-0.5 (9)
Zn1—N1—C31—C32	-73.7 (5)	C9—C4—C5—C6	1.6 (9)
Zn1—N1—C30—C28	0.1 (8)	C9—C4—C3—C2	91.9 (7)
Zn1—N2—C10—C8	2.5 (8)	C5—C4—C9—O1	177.8 (5)
Zn1—N2—C11—C20	35.8 (6)	C5—C4—C9—C8	-2.8 (9)
Zn1—N2—C11—C12	157.7 (4)	C5—C4—C3—C2	-88.6 (7)
Zn1—N2—C11—C16	-81.1 (6)	C20—C11—C12—C13	-60.3 (7)
O2—C29—C24—C25	178.8 (6)	C20—C11—C16—C15	60.9 (8)
O2—C29—C24—C23	-0.4 (9)	C20—C18—C17—C15	-60.3 (8)
N1—C31—C36—C35	-174.5 (5)	C36—C31—C37—C38	-58.4 (7)
N1—C31—C37—C38	-179.4 (5)	C36—C31—C32—C33	58.8 (6)
N1—C31—C32—C33	174.3 (5)	C36—C35—C34—C33	-60.2 (7)
N1—C30—C28—C29	5.5 (10)	C36—C35—C40—C38	58.9 (7)
N1—C30—C28—C27	-176.1 (6)	C3—C4—C9—O1	-2.7 (8)
N2—C11—C20—C18	-173.7 (5)	C3—C4—C9—C8	176.6 (5)
N2—C11—C12—C13	178.5 (5)	C3—C4—C5—C6	-177.8 (6)
N2—C11—C16—C15	176.7 (6)	C37—C31—C36—C35	59.6 (7)
C8—C7—C6—C5	-0.8 (10)	C37—C31—C32—C33	-60.2 (7)
C31—N1—C30—C28	-179.9 (5)	C37—C38—C39—C33	61.2 (7)
C31—C37—C38—C40	59.6 (7)	C27—C28—C29—O2	-176.9 (6)
C31—C37—C38—C39	-60.8 (7)	C27—C28—C29—C24	3.6 (9)
C31—C32—C33—C34	-59.9 (7)	C24—C25—C26—C27	3.1 (10)
C31—C32—C33—C39	60.4 (7)	C24—C23—C22—C21	-117.9 (16)
C30—N1—C31—C36	-137.4 (5)	C12—C11—C20—C18	61.0 (7)
C30—N1—C31—C37	-15.3 (7)	C12—C11—C16—C15	-59.1 (8)
C30—N1—C31—C32	106.2 (6)	C12—C13—C14—C15	60.1 (8)
C30—C28—C29—O2	1.4 (10)	C32—C31—C36—C35	-59.2 (6)
C30—C28—C29—C24	-178.1 (6)	C32—C31—C37—C38	60.2 (7)
C30—C28—C27—C26	179.3 (6)	C32—C33—C34—C35	60.5 (6)
C10—N2—C11—C20	-147.6 (6)	C32—C33—C39—C38	-61.0 (7)

C10—N2—C11—C12	-25.7 (8)	C34—C35—C36—C31	60.0 (7)
C10—N2—C11—C16	95.4 (7)	C34—C35—C40—C38	-60.2 (7)
C10—C8—C7—C6	-178.8 (6)	C34—C33—C39—C38	58.4 (7)
C10—C8—C9—O1	-0.3 (9)	C40—C35—C36—C31	-59.0 (6)
C10—C8—C9—C4	-179.6 (6)	C40—C35—C34—C33	58.5 (6)
C28—C29—C24—C25	-1.7 (9)	C40—C38—C39—C33	-59.5 (7)
C28—C29—C24—C23	179.1 (6)	C25—C24—C23—C22	24.0 (13)
C28—C27—C26—C25	-1.1 (10)	C39—C33—C34—C35	-58.6 (7)
C29—C28—C27—C26	-2.2 (9)	C19—C18—C17—C15	58.9 (8)
C29—C24—C25—C26	-1.7 (10)	C19—C13—C14—C15	-60.8 (7)
C29—C24—C23—C22	-156.8 (11)	C23—C24—C25—C26	177.5 (6)
C4—C5—C6—C7	0.3 (10)	C18—C19—C13—C12	-60.5 (8)
C4—C3—C2—C1	120.4 (8)	C18—C19—C13—C14	60.6 (7)
C7—C8—C10—N2	-171.8 (6)	C16—C11—C20—C18	-59.3 (7)
C7—C8—C9—O1	-178.4 (6)	C16—C11—C12—C13	59.7 (7)
C7—C8—C9—C4	2.3 (8)	C16—C15—C17—C18	61.2 (8)
C11—N2—C10—C8	-174.1 (5)	C16—C15—C14—C13	-58.9 (8)
C11—C20—C18—C19	-60.6 (7)	C13—C19—C18—C20	60.0 (7)
C11—C20—C18—C17	59.2 (8)	C13—C19—C18—C17	-59.5 (7)
C11—C12—C13—C19	60.5 (7)	C17—C15—C14—C13	59.7 (8)
C11—C12—C13—C14	-60.6 (8)	C14—C15—C17—C18	-58.6 (8)