Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Metal centre in salen-acridine dyad N_2O_2 ligand-metal complex modulates DNA binding and photocleavage efficiency

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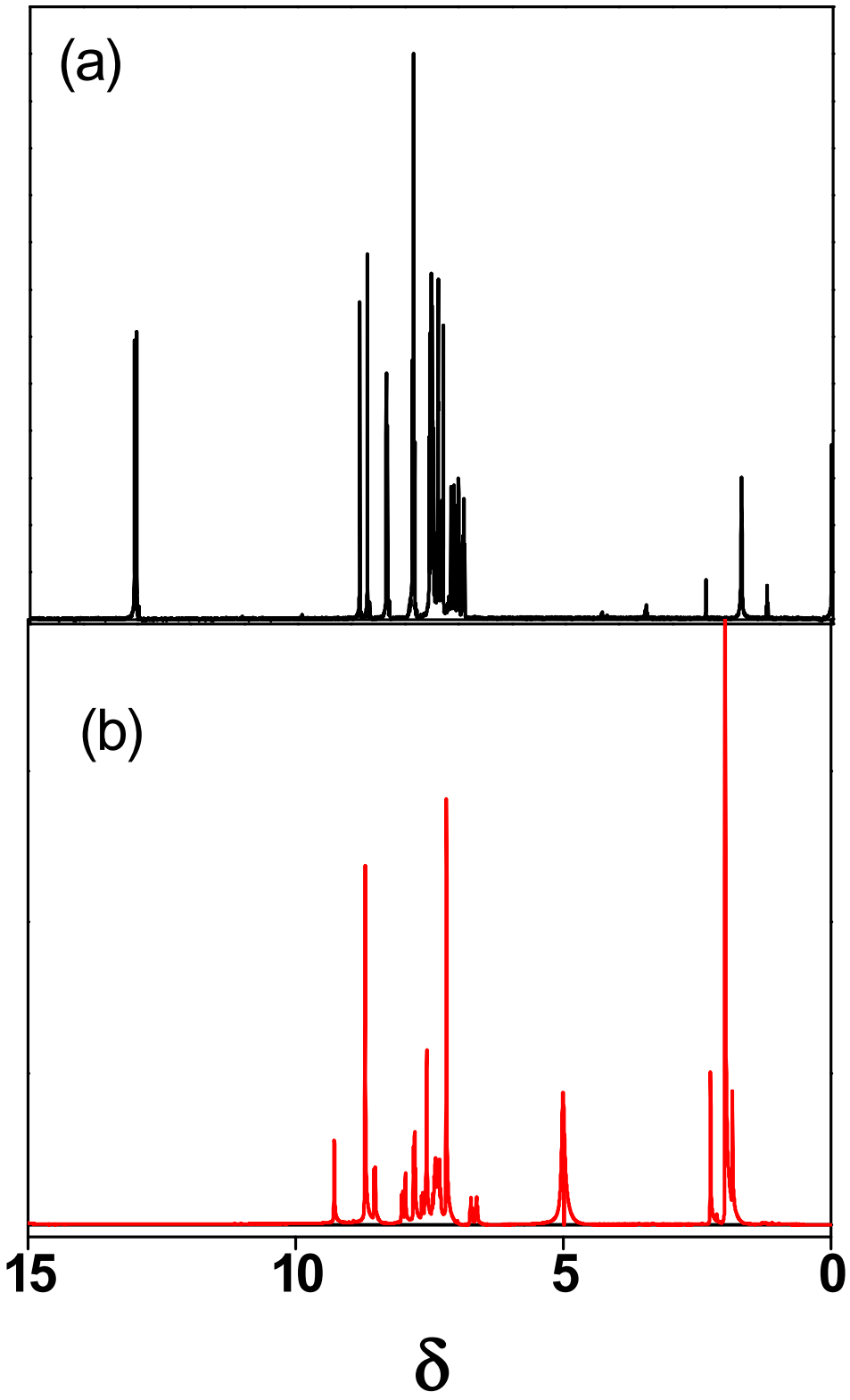

Fig. S1: ^{1}H NMR spectra of (a) H_2daasal (in $CDCl_3$) and (b) [Zn(daasal)] (in C_5D_5N).

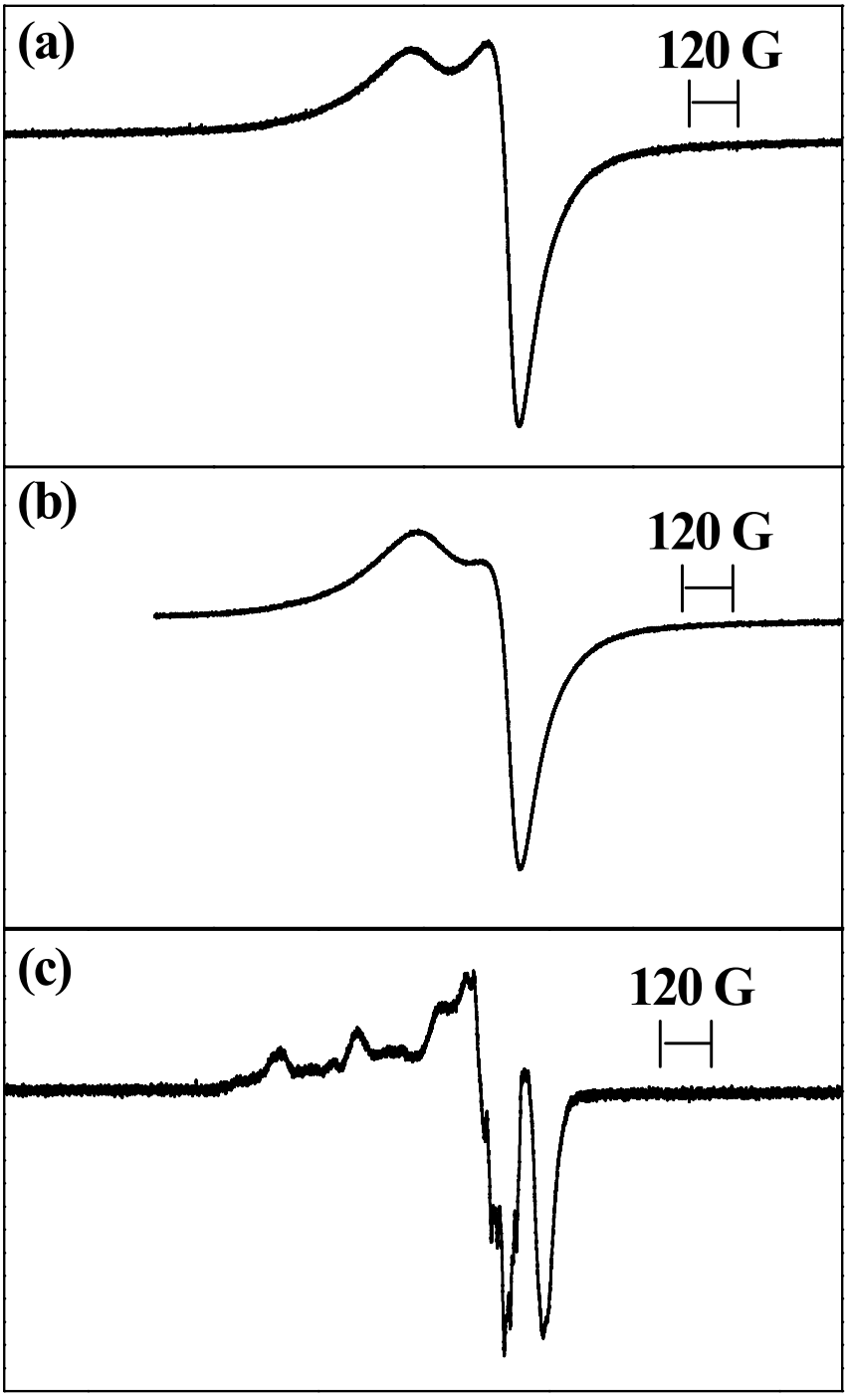

Fig. S2: ESR spectra of [Cu(daasal)] in (a) powder phase (298 K) (b) powder phase (110 K) and (c) frozen (110 K) DMF-toluene (1:1).

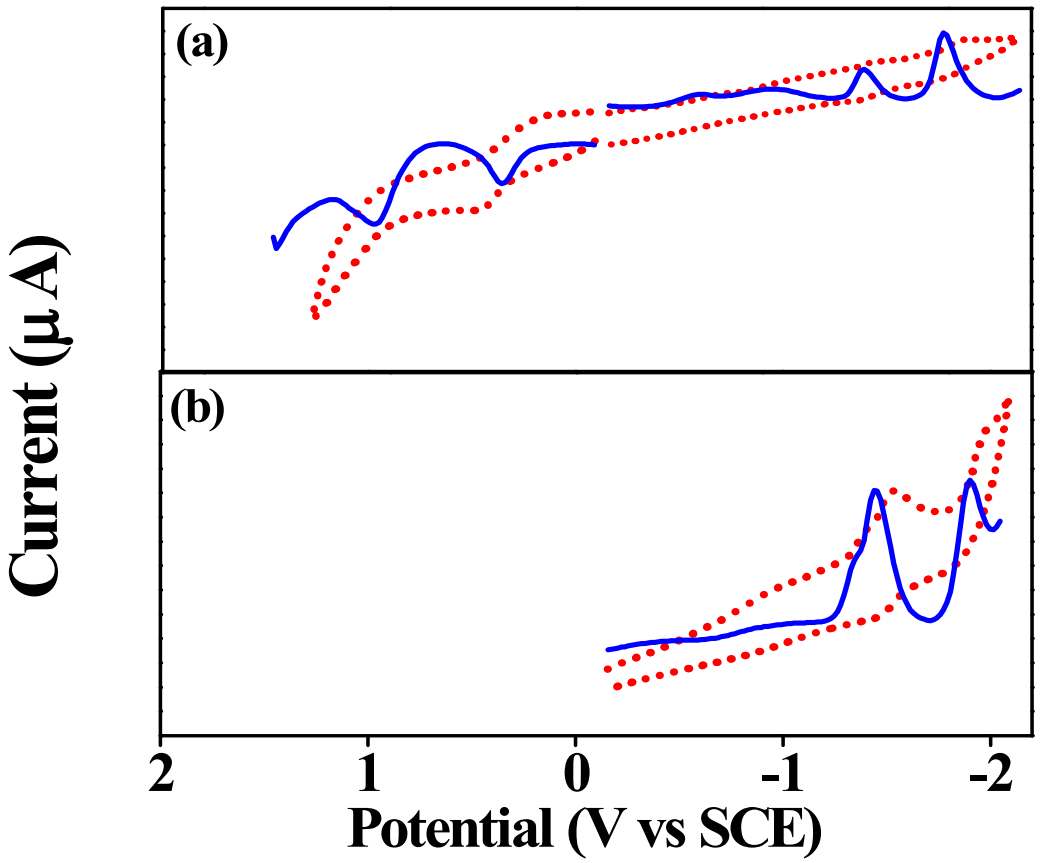

Fig. S3: Cyclic (·····) and differential pulse (——) voltammograms of (a) [Cu(daasal)] and (b) [Zn(daasal)] in CH_3CN and DMF containing 0.1 M TBAP as solvents for the anodic and cathodic runs, respectively. Scan rate: 100 mV s^{-1}.

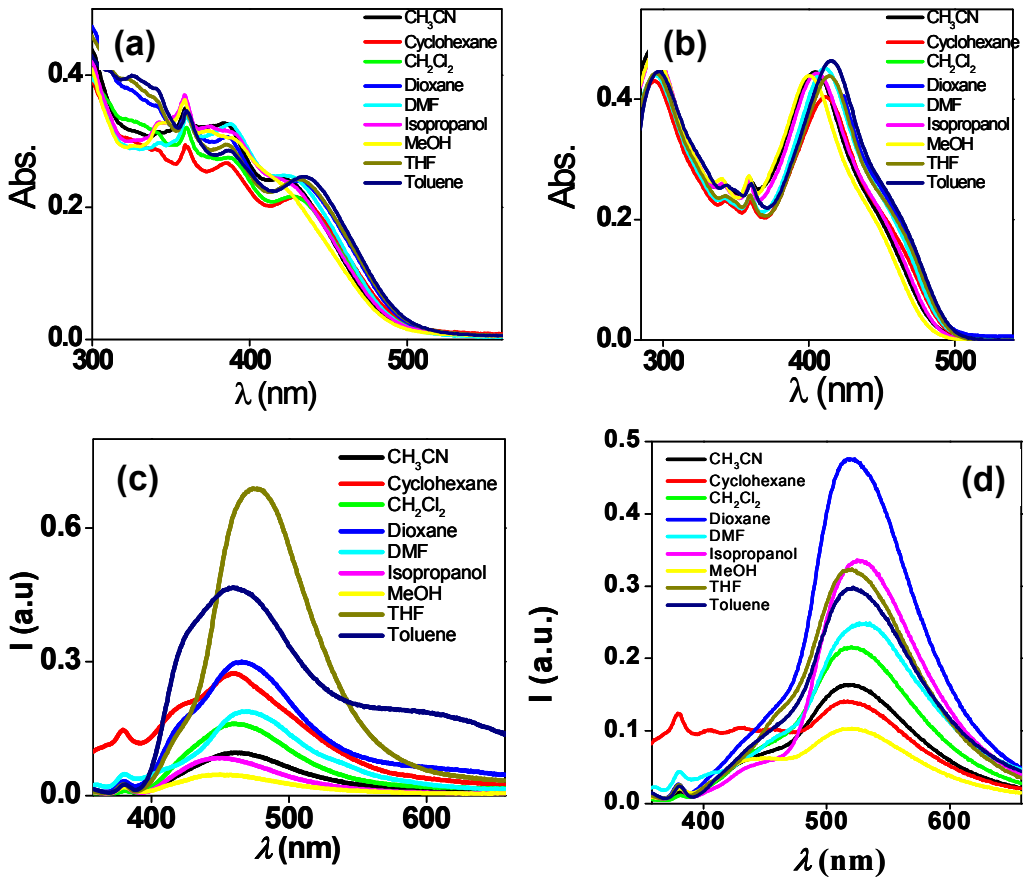

Fig. S4: Solvent dependent absorption (a, b) and emission spectra (c, d) for the compounds [Cu(daasal)] and [Zn(daasal)] at 0.2 OD. Quantum yield was calculated using the following equation

$Q_f = Q_{ref} \times a_{ref}/a_{sam} \times A_{smp}/A_{ref} \times (n_{sam}/n_{ref})^2$

where Q_f = Quantum yield of sample, Q_{ref} = Quantum yield of reference, a_{ref} = Integral area of reference, a_{sam} = Integral area of sample, A_{ref} = Absorbance of reference, A_{sam} = Absorbance of sample, n_{sam} = refractive index of the solvent (for sample), n_{ref} = refractive index of the solvent (for reference)

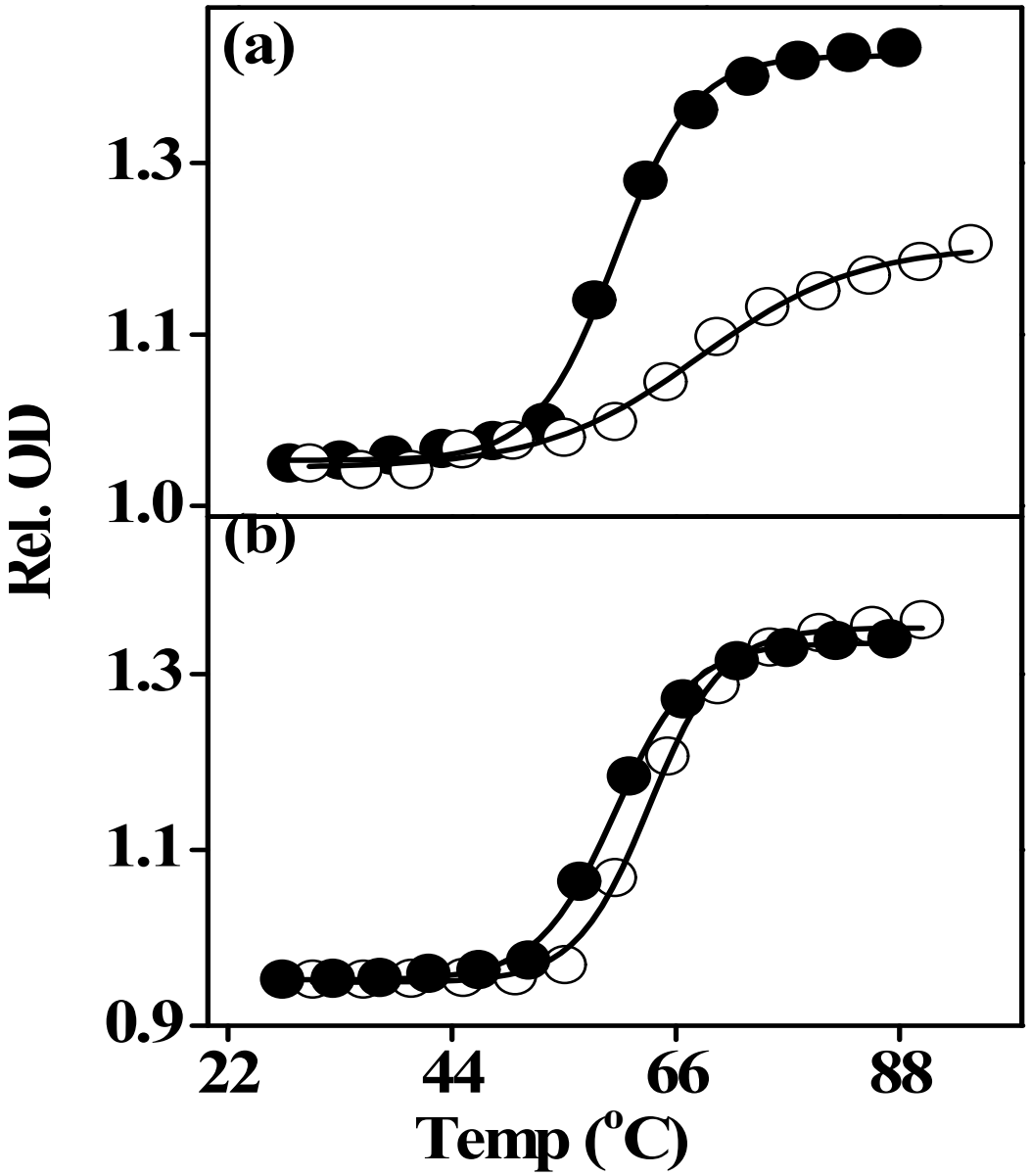

Fig. S5: Thermal melting curves of CT DNA (150 μM) in the absence (●) and in the presence (ᘓ) of (a) [Cu(daasal)] and (b) [Zn(daasal)] ([(DNA)]/ [complex] = 25) in buffer B.

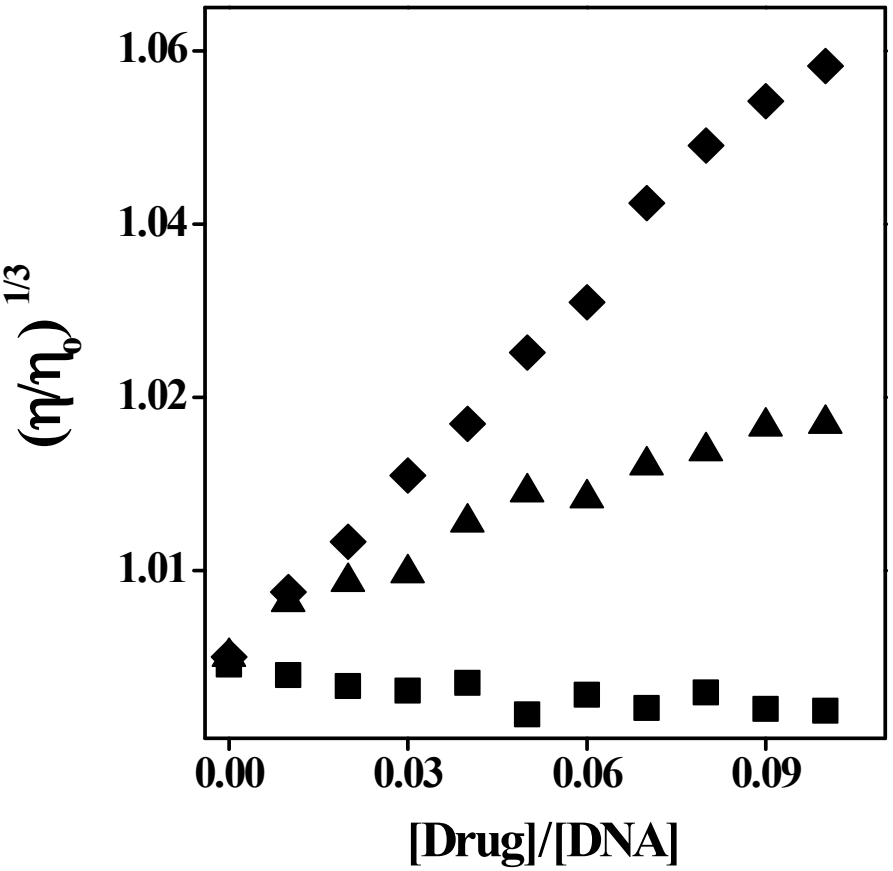

Fig. S6: Viscosity measurement for CT DNA (300 μM, Buffer C) with the complexes [Cu(daasal)] (□), [Zn(daasal)] (■) and EtBr (◴) in buffer C.

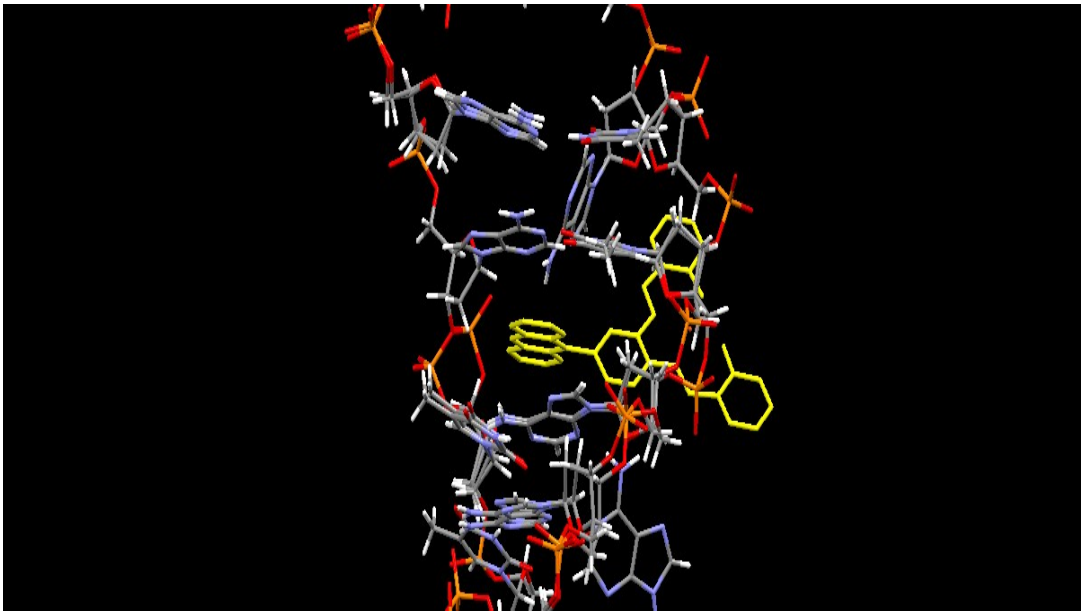

Fig. S7: Optimised structure of [Cu(daasal)] bound to the $d(CG)_{10}$ sequence in the major groove region. The heat of formation for this model is -16.33 kcal/mole

Table S1: Selected bond lengths [Å] and angles [º] for [Zn(daasal)].C_5H_5N

Zn(1)-O(1)	1.9766(13)	C(16)-N(2)-Zn(1)	112.87(11)
Zn(1)-O(2)	1.9791(13)	C(34)-N(3)-Zn(1)	120.10(13)
Zn(1)-N(1)	2.0932(15)	C(38)-N(3)-Zn(1)	121.59(12)
Zn(1)-N(2)	2.0911(14)	C(38)-N(3)-C(34)	118.01(16)
Zn(1)-N(3)	2.0860(15)	C(23)-N(4)-C(24)	118.12(15)
O(1)-C(3)	1.294(2)	N(1)-C(1)-H(1)	117.2
O(2)-C(10)	1.304(2)	N(1)-C(1)-C(2)	125.65(16)
N(1)-C(1)	1.298(2)	O(1)-C(3)-C(2)	124.37(16)
N(1)-C(15)	1.420(2)	O(1)-C(3)-C(4)	118.85(16)
N(2)-C(8)	1.299(2)	N(2)-C(8)-H(8)	117.4
N(2)-C(16)	1.417(2)	N(2)-C(8)-C(9)	125.13(16)
N(3)-C(34)	1.344(2)	O(2)-C(10)-C(9)	124.71(16)
N(3)-C(38)	1.340(2)	O(2)-C(10)-C(11)	118.37(16)
N(4)-C(23)	1.344(2)	C(16)-C(15)-N(1)	116.01(15)
N(4)-C(24)	1.346(2)	C(20)-C(15)-N(1)	124.52(16)
O(1)-Zn(1)-O(2)	93.46(5)	C(15)-C(16)-N(2)	115.62(15)
O(1)-Zn(1)-N(1)	89.02(5)	C(17)-C(16)-N(2)	125.14(16)
O(1)-Zn(1)-N(2)	157.98(6)	C(18)-C(19)-C(21)	119.79(16)
O(1)-Zn(1)-N(3)	98.62(6)	C(20)-C(19)-C(21)	120.92(16)
O(2)-Zn(1)-N(1)	151.70(6)	C(22)-C(21)-C(19)	120.40(16)
O(2)-Zn(1)-N(2)	89.29(5)	N(4)-C(23)-C(22)	123.47(16)
O(2)-Zn(1)-N(3)	101.56(6)	N(4)-C(23)-C(29)	117.84(16)
N(2)-Zn(1)-N(1)	78.54(6)	N(4)-C(24)-C(25)	123.06(17)
N(3)-Zn(1)-N(1)	105.92(6)	N(4)-C(24)-C(30)	118.34(16)
N(3)-Zn(1)-N(2)	102.22(6)	N(3)-C(34)-H(34)	118.8
C(3)-O(1)-Zn(1)	130.67(12)	N(3)-C(34)-C(35)	122.39(18)
C(10)-O(2)-Zn(1)	129.68(11)	N(3)-C(38)-C(37)	123.32(18)
C(1)-N(1)-Zn(1)	125.92(12)	N(3)-C(38)-H(38)	118.3
C(1)-N(1)-C(15)	121.17(15)		
C(15)-N(1)-Zn(1)	112.83(11)		
C(8)-N(2)-Zn(1)	126.26(12)		
C(8)-N(2)-C(16)	120.70(15)		

Table S2: Redox potential data

Compound	**Oxidation[b]** $E_{1/2}$ **(V vs SCE)**	**Reduction[c]** $E_{1/2}$ **(V vs SCE)**
acridine	---	-1.46
daa	+ 0.88, +1.40[d]	-0.77, -1.07[d]
salicylaldehyde	---	-1.82
H_2daasal*	---	- 1.44
[Ni(daasal)] *	+1.03	-1.21, -1.48
[Cu(daasal)]	+0.96	-1.35, -1.76
[Zn(daasal)]	---	-1.45, -1.91

a) Obtained from the differential pulse voltammetri measurements. Error limits: $E_{1/2,} \pm 0.03$ V, 0.1 M TBAP

b) CH_3CN

c) DMF

d) CH_2Cl_2

* M. Mariappan, M. Suenaga, A. Mukhopadhyay, B. G. Maiya, Inorg. Chim. Acta 390 (2012) 95–104

Appendix

Table A1: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 ×10^3) for MMB_180511_V_ZnH2LSal. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn(1)	9801(1)	6966(1)	6749(1)	13(1)
O(1)	11400(1)	6713(1)	8115(1)	18(1)
O(2)	10856(1)	7437(1)	6326(1)	17(1)
N(1)	8914(2)	6344(1)	6438(1)	13(1)
N(2)	8306(2)	7042(1)	4911(1)	13(1)
N(3)	8970(2)	7296(1)	7941(2)	16(1)
N(4)	2519(2)	4967(1)	3182(1)	16(1)
C(1)	9407(2)	5994(1)	7111(2)	14(1)
C(2)	10693(2)	5964(1)	8154(2)	14(1)
C(3)	11619(2)	6322(1)	8595(2)	14(1)
C(4)	12860(2)	6233(1)	9631(2)	17(1)
C(5)	13150(2)	5826(1)	10195(2)	18(1)
C(6)	12230(2)	5477(1)	9766(2)	18(1)
C(7)	11029(2)	5549(1)	8758(2)	16(1)
C(8)	8296(2)	7331(1)	4044(2)	13(1)
C(9)	9327(2)	7653(1)	4196(2)	13(1)
C(10)	10529(2)	7693(1)	5313(2)	14(1)
C(11)	11436(2)	8032(1)	5297(2)	19(1)
C(12)	11207(2)	8300(1)	4239(2)	21(1)
C(13)	10043(2)	8250(1)	3122(2)	19(1)
C(14)	9123(2)	7934(1)	3122(2)	16(1)
C(15)	7631(2)	6338(1)	5421(2)	13(1)
C(16)	7293(2)	6715(1)	4625(2)	13(1)
C(17)	6027(2)	6739(1)	3628(2)	14(1)
C(18)	5121(2)	6395(1)	3415(2)	15(1)
C(19)	5462(2)	6017(1)	4180(2)	14(1)

C(20)	6713(2)	5992(1)	5175(2)	15(1)
C(21)	4486(2)	5644(1)	3907(2)	14(1)
C(22)	4704(2)	5262(1)	3291(2)	14(1)
C(23)	3660(2)	4935(1)	2922(2)	14(1)
C(24)	2362(2)	5319(1)	3848(2)	15(1)
C(25)	3321(2)	5672(1)	4230(2)	14(1)
C(26)	5891(2)	5185(1)	2998(2)	18(1)
C(27)	6032(2)	4814(1)	2381(2)	21(1)
C(28)	4984(2)	4496(1)	1984(2)	21(1)
C(29)	3837(2)	4555(1)	2246(2)	18(1)
C(30)	1193(2)	5341(1)	4197(2)	19(1)
C(31)	1002(2)	5680(1)	4904(2)	22(1)
C(32)	1964(2)	6028(1)	5305(2)	22(1)
C(33)	3072(2)	6025(1)	4962(2)	17(1)
C(34)	9539(2)	7259(1)	9240(2)	20(1)
C(35)	9107(2)	7501(1)	10073(2)	25(1)
C(36)	8046(2)	7791(1)	9554(2)	24(1)
C(37)	7454(2)	7833(1)	8218(2)	22(1)
C(38)	7949(2)	7580(1)	7454(2)	20(1)
C(39)	9148(2)	6355(1)	2540(2)	23(1)
N(40)	10133(2)	6357(1)	2048(2)	25(1)
C(41)	10101(2)	6034(1)	1216(2)	24(1)
C(42)	9120(2)	5712(1)	851(2)	24(1)
C(43)	8100(2)	5722(1)	1353(2)	23(1)
C(44)	8121(2)	6051(1)	2220(2)	24(1)

Table A2. Bond lengths [Å] and angles [°] for MMB_180511_V_ZnH2LSal.

Zn(1)-O(1)	1.9766(13)
Zn(1)-O(2)	1.9791(13)
Zn(1)-N(1)	2.0932(15)
Zn(1)-N(2)	2.0911(14)
Zn(1)-N(3)	2.0860(15)
O(1)-C(3)	1.294(2)
O(2)-C(10)	1.304(2)
N(1)-C(1)	1.298(2)
N(1)-C(15)	1.420(2)
N(2)-C(8)	1.299(2)
N(2)-C(16)	1.417(2)
N(3)-C(34)	1.344(2)
N(3)-C(38)	1.340(2)
N(4)-C(23)	1.344(2)
N(4)-C(24)	1.346(2)
C(1)-H(1)	0.9500
C(1)-C(2)	1.438(2)
C(2)-C(3)	1.432(2)
C(2)-C(7)	1.417(2)
C(3)-C(4)	1.426(2)
C(4)-H(4)	0.9500
C(4)-C(5)	1.373(3)
C(5)-H(5)	0.9500
C(5)-C(6)	1.406(3)
C(6)-H(6)	0.9500
C(6)-C(7)	1.375(3)
C(7)-H(7)	0.9500
C(8)-H(8)	0.9500
C(8)-C(9)	1.435(2)
C(9)-C(10)	1.425(2)
C(9)-C(14)	1.415(2)
C(10)-C(11)	1.418(2)

C(11)-H(11)	0.9500
C(11)-C(12)	1.373(3)
C(12)-H(12)	0.9500
C(12)-C(13)	1.405(3)
C(13)-H(13)	0.9500
C(13)-C(14)	1.373(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.413(2)
C(15)-C(20)	1.396(2)
C(16)-C(17)	1.399(2)
C(17)-H(17)	0.9500
C(17)-C(18)	1.384(2)
C(18)-H(18)	0.9500
C(18)-C(19)	1.399(2)
C(19)-C(20)	1.388(3)
C(19)-C(21)	1.495(2)
C(20)-H(20)	0.9500
C(21)-C(22)	1.409(2)
C(21)-C(25)	1.407(3)
C(22)-C(23)	1.438(2)
C(22)-C(26)	1.428(3)
C(23)-C(29)	1.428(2)
C(24)-C(25)	1.438(2)
C(24)-C(30)	1.426(3)
C(25)-C(33)	1.427(2)
C(26)-H(26)	0.9500
C(26)-C(27)	1.358(3)
C(27)-H(27)	0.9500
C(27)-C(28)	1.422(3)
C(28)-H(28)	0.9500
C(28)-C(29)	1.361(3)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(30)-C(31)	1.355(3)

C(31)-H(31)	0.9500
C(31)-C(32)	1.427(3)
C(32)-H(32)	0.9500
C(32)-C(33)	1.359(3)
C(33)-H(33)	0.9500
C(34)-H(34)	0.9500
C(34)-C(35)	1.380(3)
C(35)-H(35)	0.9500
C(35)-C(36)	1.385(3)
C(36)-H(36)	0.9500
C(36)-C(37)	1.384(3)
C(37)-H(37)	0.9500
C(37)-C(38)	1.379(3)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(39)-N(40)	1.339(3)
C(39)-C(44)	1.378(3)
N(40)-C(41)	1.339(3)
C(41)-H(41)	0.9500
C(41)-C(42)	1.383(3)
C(42)-H(42)	0.9500
C(42)-C(43)	1.382(3)
C(43)-H(43)	0.9500
C(43)-C(44)	1.381(3)
C(44)-H(44)	0.9500

O(1)-Zn(1)-O(2)	93.46(5)
O(1)-Zn(1)-N(1)	89.02(5)
O(1)-Zn(1)-N(2)	157.98(6)
O(1)-Zn(1)-N(3)	98.62(6)
O(2)-Zn(1)-N(1)	151.70(6)
O(2)-Zn(1)-N(2)	89.29(5)
O(2)-Zn(1)-N(3)	101.56(6)
N(2)-Zn(1)-N(1)	78.54(6)

N(3)-Zn(1)-N(1)	105.92(6)
N(3)-Zn(1)-N(2)	102.22(6)
C(3)-O(1)-Zn(1)	130.67(12)
C(10)-O(2)-Zn(1)	129.68(11)
C(1)-N(1)-Zn(1)	125.92(12)
C(1)-N(1)-C(15)	121.17(15)
C(15)-N(1)-Zn(1)	112.83(11)
C(8)-N(2)-Zn(1)	126.26(12)
C(8)-N(2)-C(16)	120.70(15)
C(16)-N(2)-Zn(1)	112.87(11)
C(34)-N(3)-Zn(1)	120.10(13)
C(38)-N(3)-Zn(1)	121.59(12)
C(38)-N(3)-C(34)	118.01(16)
C(23)-N(4)-C(24)	118.12(15)
N(1)-C(1)-H(1)	117.2
N(1)-C(1)-C(2)	125.65(16)
C(2)-C(1)-H(1)	117.2
C(3)-C(2)-C(1)	124.11(16)
C(7)-C(2)-C(1)	116.11(16)
C(7)-C(2)-C(3)	119.79(16)
O(1)-C(3)-C(2)	124.37(16)
O(1)-C(3)-C(4)	118.85(16)
C(4)-C(3)-C(2)	116.77(16)
C(3)-C(4)-H(4)	119.1
C(5)-C(4)-C(3)	121.81(17)
C(5)-C(4)-H(4)	119.1
C(4)-C(5)-H(5)	119.5
C(4)-C(5)-C(6)	121.10(17)
C(6)-C(5)-H(5)	119.5
C(5)-C(6)-H(6)	120.6
C(7)-C(6)-C(5)	118.85(17)
C(7)-C(6)-H(6)	120.6
C(2)-C(7)-H(7)	119.2
C(6)-C(7)-C(2)	121.68(17)

C(6)-C(7)-H(7)	119.2
N(2)-C(8)-H(8)	117.4
N(2)-C(8)-C(9)	125.13(16)
C(9)-C(8)-H(8)	117.4
C(10)-C(9)-C(8)	124.62(16)
C(14)-C(9)-C(8)	115.86(16)
C(14)-C(9)-C(10)	119.48(16)
O(2)-C(10)-C(9)	124.71(16)
O(2)-C(10)-C(11)	118.37(16)
C(11)-C(10)-C(9)	116.91(16)
C(10)-C(11)-H(11)	118.9
C(12)-C(11)-C(10)	122.12(17)
C(12)-C(11)-H(11)	118.9
C(11)-C(12)-H(12)	119.6
C(11)-C(12)-C(13)	120.80(17)
C(13)-C(12)-H(12)	119.6
C(12)-C(13)-H(13)	120.7
C(14)-C(13)-C(12)	118.53(17)
C(14)-C(13)-H(13)	120.7
C(9)-C(14)-H(14)	119.0
C(13)-C(14)-C(9)	122.09(17)
C(13)-C(14)-H(14)	119.0
C(16)-C(15)-N(1)	116.01(15)
C(20)-C(15)-N(1)	124.52(16)
C(20)-C(15)-C(16)	119.47(16)
C(15)-C(16)-N(2)	115.62(15)
C(17)-C(16)-N(2)	125.14(16)
C(17)-C(16)-C(15)	119.24(16)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-C(16)	120.42(16)
C(18)-C(17)-H(17)	119.8
C(17)-C(18)-H(18)	119.7
C(17)-C(18)-C(19)	120.61(17)
C(19)-C(18)-H(18)	119.7

C(18)-C(19)-C(21)	119.79(16)
C(20)-C(19)-C(18)	119.28(16)
C(20)-C(19)-C(21)	120.92(16)
C(15)-C(20)-H(20)	119.5
C(19)-C(20)-C(15)	120.94(16)
C(19)-C(20)-H(20)	119.5
C(22)-C(21)-C(19)	120.40(16)
C(25)-C(21)-C(19)	120.69(16)
C(25)-C(21)-C(22)	118.89(16)
C(21)-C(22)-C(23)	117.90(16)
C(21)-C(22)-C(26)	123.82(17)
C(26)-C(22)-C(23)	118.27(16)
N(4)-C(23)-C(22)	123.47(16)
N(4)-C(23)-C(29)	117.84(16)
C(29)-C(23)-C(22)	118.69(16)
N(4)-C(24)-C(25)	123.06(17)
N(4)-C(24)-C(30)	118.34(16)
C(30)-C(24)-C(25)	118.60(16)
C(21)-C(25)-C(24)	118.32(16)
C(21)-C(25)-C(33)	123.14(17)
C(33)-C(25)-C(24)	118.49(17)
C(22)-C(26)-H(26)	119.4
C(27)-C(26)-C(22)	121.12(18)
C(27)-C(26)-H(26)	119.4
C(26)-C(27)-H(27)	119.7
C(26)-C(27)-C(28)	120.66(18)
C(28)-C(27)-H(27)	119.7
C(27)-C(28)-H(28)	119.9
C(29)-C(28)-C(27)	120.25(17)
C(29)-C(28)-H(28)	119.9
C(23)-C(29)-H(29)	119.5
C(28)-C(29)-C(23)	120.97(17)

C(28)-C(29)-H(29)	119.5
C(24)-C(30)-H(30)	119.5
C(31)-C(30)-C(24)	120.99(18)
C(31)-C(30)-H(30)	119.5
C(30)-C(31)-H(31)	119.7
C(30)-C(31)-C(32)	120.58(18)
C(32)-C(31)-H(31)	119.7
C(31)-C(32)-H(32)	119.9
C(33)-C(32)-C(31)	120.25(18)
C(33)-C(32)-H(32)	119.9
C(25)-C(33)-H(33)	119.5
C(32)-C(33)-C(25)	121.05(17)
C(32)-C(33)-H(33)	119.5
N(3)-C(34)-H(34)	118.8
N(3)-C(34)-C(35)	122.39(18)
C(35)-C(34)-H(34)	118.8
C(34)-C(35)-H(35)	120.6
C(34)-C(35)-C(36)	118.83(19)
C(36)-C(35)-H(35)	120.6
C(35)-C(36)-H(36)	120.3
C(37)-C(36)-C(35)	119.37(18)
C(37)-C(36)-H(36)	120.3
C(36)-C(37)-H(37)	121.0
C(38)-C(37)-C(36)	118.08(19)
C(38)-C(37)-H(37)	121.0
N(3)-C(38)-C(37)	123.32(18)
N(3)-C(38)-H(38)	118.3
C(37)-C(38)-H(38)	118.3
N(40)-C(39)-H(39)	118.0
N(40)-C(39)-C(44)	124.02(18)
C(44)-C(39)-H(39)	118.0
C(39)-N(40)-C(41)	116.32(17)
N(40)-C(41)-H(41)	118.2
N(40)-C(41)-C(42)	123.66(19)

C(42)-C(41)-H(41)	118.2
C(41)-C(42)-H(42)	120.6
C(43)-C(42)-C(41)	118.88(18)
C(43)-C(42)-H(42)	120.6
C(42)-C(43)-H(43)	120.8
C(44)-C(43)-C(42)	118.31(19)
C(44)-C(43)-H(43)	120.8
C(39)-C(44)-C(43)	118.77(19)
C(39)-C(44)-H(44)	120.6
C(43)-C(44)-H(44)	120.6

Symmetry transformations used to generate equivalent atoms:

Table A3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for MMB_180511_V_ZnH2LSal. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	14(1)	11(1)	11(1)	1(1)	2(1)	0(1)
O(1)	17(1)	14(1)	19(1)	5(1)	1(1)	-1(1)
O(2)	17(1)	18(1)	13(1)	4(1)	0(1)	-4(1)
N(1)	14(1)	12(1)	12(1)	1(1)	4(1)	0(1)
N(2)	14(1)	12(1)	11(1)	-1(1)	3(1)	0(1)
N(3)	17(1)	16(1)	15(1)	-1(1)	6(1)	-2(1)
N(4)	17(1)	13(1)	15(1)	1(1)	4(1)	-1(1)
C(1)	17(1)	12(1)	14(1)	0(1)	6(1)	-1(1)
C(2)	16(1)	15(1)	11(1)	1(1)	6(1)	3(1)
C(3)	15(1)	17(1)	12(1)	2(1)	6(1)	3(1)
C(4)	17(1)	19(1)	14(1)	1(1)	4(1)	0(1)
C(5)	16(1)	24(1)	13(1)	2(1)	3(1)	5(1)
C(6)	24(1)	16(1)	16(1)	4(1)	8(1)	5(1)
C(7)	20(1)	14(1)	15(1)	0(1)	7(1)	1(1)
C(8)	13(1)	14(1)	10(1)	-2(1)	2(1)	2(1)
C(9)	15(1)	13(1)	12(1)	-1(1)	5(1)	1(1)
C(10)	16(1)	13(1)	13(1)	-1(1)	4(1)	1(1)
C(11)	19(1)	19(1)	17(1)	0(1)	2(1)	-5(1)
C(12)	22(1)	17(1)	23(1)	1(1)	8(1)	-6(1)
C(13)	24(1)	17(1)	16(1)	4(1)	7(1)	-1(1)
C(14)	19(1)	16(1)	13(1)	0(1)	4(1)	1(1)
C(15)	14(1)	15(1)	11(1)	-2(1)	4(1)	1(1)
C(16)	15(1)	12(1)	13(1)	-2(1)	6(1)	0(1)
C(17)	17(1)	12(1)	13(1)	1(1)	4(1)	2(1)
C(18)	13(1)	15(1)	14(1)	-2(1)	2(1)	1(1)
C(19)	15(1)	14(1)	15(1)	-2(1)	6(1)	0(1)
C(20)	18(1)	13(1)	13(1)	1(1)	6(1)	-1(1)

C(21)	15(1)	14(1)	11(1)	3(1)	2(1)	1(1)
C(22)	16(1)	14(1)	10(1)	4(1)	4(1)	2(1)
C(23)	16(1)	14(1)	11(1)	3(1)	3(1)	0(1)
C(24)	16(1)	13(1)	13(1)	3(1)	3(1)	0(1)
C(25)	16(1)	13(1)	12(1)	1(1)	3(1)	0(1)
C(26)	19(1)	17(1)	19(1)	1(1)	8(1)	-2(1)
C(27)	24(1)	20(1)	22(1)	1(1)	13(1)	3(1)
C(28)	31(1)	14(1)	20(1)	-1(1)	12(1)	3(1)
C(29)	23(1)	14(1)	16(1)	0(1)	7(1)	-3(1)
C(30)	18(1)	18(1)	22(1)	2(1)	8(1)	-2(1)
C(31)	19(1)	25(1)	24(1)	2(1)	13(1)	2(1)
C(32)	26(1)	19(1)	21(1)	-2(1)	11(1)	3(1)
C(33)	21(1)	14(1)	16(1)	-1(1)	6(1)	-1(1)
C(34)	23(1)	21(1)	16(1)	2(1)	5(1)	1(1)
C(35)	32(1)	27(1)	17(1)	-1(1)	10(1)	1(1)
C(36)	31(1)	21(1)	26(1)	-4(1)	17(1)	-1(1)
C(37)	22(1)	19(1)	28(1)	1(1)	10(1)	3(1)
C(38)	20(1)	21(1)	18(1)	1(1)	5(1)	1(1)
C(39)	28(1)	20(1)	23(1)	-2(1)	9(1)	5(1)
N(40)	26(1)	24(1)	26(1)	-3(1)	11(1)	-3(1)
C(41)	26(1)	26(1)	26(1)	-1(1)	14(1)	-1(1)
C(42)	29(1)	21(1)	23(1)	-4(1)	12(1)	-1(1)
C(43)	24(1)	20(1)	26(1)	1(1)	9(1)	-3(1)
C(44)	25(1)	23(1)	27(1)	4(1)	15(1)	5(1)

Table A4. Hydrogen coordinates (× 10^4) and isotropic displacement parameters (Å^2 × 10^3) for MMB_180511_V_ZnH2LSal.

	x	y	z	U(eq)
H(1)	8872	5736	6896	17
H(4)	13505	6461	9940	21
H(5)	13985	5779	10886	22
H(6)	12435	5198	10166	22
H(7)	10408	5313	8458	20
H(8)	7547	7330	3247	15
H(11)	12228	8076	6042	23
H(12)	11844	8522	4262	25
H(13)	9894	8432	2384	23
H(14)	8325	7903	2376	20
H(17)	5787	6992	3095	17
H(18)	4260	6417	2743	18
H(20)	6949	5736	5696	18
H(26)	6593	5397	3239	22
H(27)	6838	4766	2213	25
H(28)	5085	4241	1533	25
H(29)	3143	4340	1976	21
H(30)	538	5114	3930	23
H(31)	222	5687	5134	26
H(32)	1829	6261	5814	26
H(33)	3692	6262	5213	21
H(34)	10265	7059	9596	24
H(35)	9531	7470	10988	30
H(36)	7726	7960	10108	29
H(37)	6728	8031	7838	27
H(38)	7546	7608	6537	24
H(39)	9159	6577	3147	28

H(41)	10791	6025	856	29
H(42)	9147	5487	265	28
H(43)	7402	5509	1107	28
H(44)	7439	6067	2589	28

Table A5: Torsion angles [°] for MMB_180511_V_ZnH2LSal.

Zn(1)-O(1)-C(3)-C(2)	3.2(3)
Zn(1)-O(1)-C(3)-C(4)	-177.12(12)
Zn(1)-O(2)-C(10)-C(9)	-6.3(3)
Zn(1)-O(2)-C(10)-C(11)	174.78(13)
Zn(1)-N(1)-C(1)-C(2)	-3.7(3)
Zn(1)-N(1)-C(15)-C(16)	12.68(18)
Zn(1)-N(1)-C(15)-C(20)	-167.15(14)
Zn(1)-N(2)-C(8)-C(9)	0.3(2)
Zn(1)-N(2)-C(16)-C(15)	-16.69(18)
Zn(1)-N(2)-C(16)-C(17)	163.95(14)
Zn(1)-N(3)-C(34)-C(35)	173.84(15)
Zn(1)-N(3)-C(38)-C(37)	-173.91(15)
O(1)-C(3)-C(4)-C(5)	179.27(17)
O(2)-C(10)-C(11)-C(12)	176.23(18)
N(1)-C(1)-C(2)-C(3)	0.0(3)
N(1)-C(1)-C(2)-C(7)	179.91(17)
N(1)-C(15)-C(16)-N(2)	2.6(2)
N(1)-C(15)-C(16)-C(17)	-177.96(15)
N(1)-C(15)-C(20)-C(19)	178.26(16)
N(2)-C(8)-C(9)-C(10)	1.7(3)
N(2)-C(8)-C(9)-C(14)	179.22(16)
N(2)-C(16)-C(17)-C(18)	178.62(16)
N(3)-C(34)-C(35)-C(36)	0.3(3)
N(4)-C(23)-C(29)-C(28)	-178.13(17)
N(4)-C(24)-C(25)-C(21)	-1.0(3)
N(4)-C(24)-C(25)-C(33)	-178.48(16)
N(4)-C(24)-C(30)-C(31)	177.84(17)
C(1)-N(1)-C(15)-C(16)	-170.30(16)
C(1)-N(1)-C(15)-C(20)	9.9(3)
C(1)-C(2)-C(3)-O(1)	0.5(3)
C(1)-C(2)-C(3)-C(4)	-179.19(16)
C(1)-C(2)-C(7)-C(6)	180.00(17)

C(2)-C(3)-C(4)-C(5)	-1.0(3)
C(3)-C(2)-C(7)-C(6)	-0.1(3)
C(3)-C(4)-C(5)-C(6)	0.3(3)
C(4)-C(5)-C(6)-C(7)	0.5(3)
C(5)-C(6)-C(7)-C(2)	-0.7(3)
C(7)-C(2)-C(3)-O(1)	-179.41(16)
C(7)-C(2)-C(3)-C(4)	0.9(2)
C(8)-N(2)-C(16)-C(15)	158.93(16)
C(8)-N(2)-C(16)-C(17)	-20.4(3)
C(8)-C(9)-C(10)-O(2)	1.3(3)
C(8)-C(9)-C(10)-C(11)	-179.75(17)
C(8)-C(9)-C(14)-C(13)	-178.55(17)
C(9)-C(10)-C(11)-C(12)	-2.7(3)
C(10)-C(9)-C(14)-C(13)	-0.9(3)
C(10)-C(11)-C(12)-C(13)	0.7(3)
C(11)-C(12)-C(13)-C(14)	1.4(3)
C(12)-C(13)-C(14)-C(9)	-1.2(3)
C(14)-C(9)-C(10)-O(2)	-176.10(17)
C(14)-C(9)-C(10)-C(11)	2.8(2)
C(15)-N(1)-C(1)-C(2)	179.73(16)
C(15)-C(16)-C(17)-C(18)	-0.7(3)
C(16)-N(2)-C(8)-C(9)	-174.71(16)
C(16)-C(15)-C(20)-C(19)	-1.6(3)
C(16)-C(17)-C(18)-C(19)	-0.8(3)
C(17)-C(18)-C(19)-C(20)	1.1(3)
C(17)-C(18)-C(19)-C(21)	-178.03(16)
C(18)-C(19)-C(20)-C(15)	0.1(3)
C(18)-C(19)-C(21)-C(22)	104.9(2)
C(18)-C(19)-C(21)-C(25)	-73.5(2)
C(19)-C(21)-C(22)-C(23)	-173.16(15)
C(19)-C(21)-C(22)-C(26)	5.9(3)
C(19)-C(21)-C(25)-C(24)	174.91(15)
C(19)-C(21)-C(25)-C(33)	-7.7(3)
C(20)-C(15)-C(16)-N(2)	-177.52(15)

C(20)-C(15)-C(16)-C(17)	1.9(3)
C(20)-C(19)-C(21)-C(22)	-74.2(2)
C(20)-C(19)-C(21)-C(25)	107.3(2)
C(21)-C(19)-C(20)-C(15)	179.21(16)
C(21)-C(22)-C(23)-N(4)	-2.9(3)
C(21)-C(22)-C(23)-C(29)	177.30(16)
C(21)-C(22)-C(26)-C(27)	-178.76(17)
C(21)-C(25)-C(33)-C(32)	-176.72(18)
C(22)-C(21)-C(25)-C(24)	-3.5(2)
C(22)-C(21)-C(25)-C(33)	173.88(16)
C(22)-C(23)-C(29)-C(28)	1.7(3)
C(22)-C(26)-C(27)-C(28)	1.4(3)
C(23)-N(4)-C(24)-C(25)	3.5(3)
C(23)-N(4)-C(24)-C(30)	-176.13(16)
C(23)-C(22)-C(26)-C(27)	0.3(3)
C(24)-N(4)-C(23)-C(22)	-1.5(3)
C(24)-N(4)-C(23)-C(29)	178.31(16)
C(24)-C(25)-C(33)-C(32)	0.7(3)
C(24)-C(30)-C(31)-C(32)	0.6(3)
C(25)-C(21)-C(22)-C(23)	5.3(2)
C(25)-C(21)-C(22)-C(26)	-175.61(16)
C(25)-C(24)-C(30)-C(31)	-1.8(3)
C(26)-C(22)-C(23)-N(4)	177.96(16)
C(26)-C(22)-C(23)-C(29)	-1.9(2)
C(26)-C(27)-C(28)-C(29)	-1.6(3)
C(27)-C(28)-C(29)-C(23)	0.0(3)
C(30)-C(24)-C(25)-C(21)	178.64(16)
C(30)-C(24)-C(25)-C(33)	1.1(2)
C(30)-C(31)-C(32)-C(33)	1.2(3)
C(31)-C(32)-C(33)-C(25)	-1.8(3)
C(34)-N(3)-C(38)-C(37)	-0.3(3)
C(34)-C(35)-C(36)-C(37)	-0.5(3)
C(35)-C(36)-C(37)-C(38)	0.4(3)
C(36)-C(37)-C(38)-N(3)	0.0(3)

C(38)-N(3)-C(34)-C(35)	0.1(3)
C(39)-N(40)-C(41)-C(42)	0.5(3)
N(40)-C(39)-C(44)-C(43)	0.9(3)
N(40)-C(41)-C(42)-C(43)	0.8(3)
C(41)-C(42)-C(43)-C(44)	-1.2(3)
C(42)-C(43)-C(44)-C(39)	0.5(3)
C(44)-C(39)-N(40)-C(41)	-1.3(3)

Symmetry transformations used to generate equivalent atoms: