Absorption and anti-bacterial studies of acetylene functionalized Schiff base for recognition of Sn (II) and inhibition of *E. coli*

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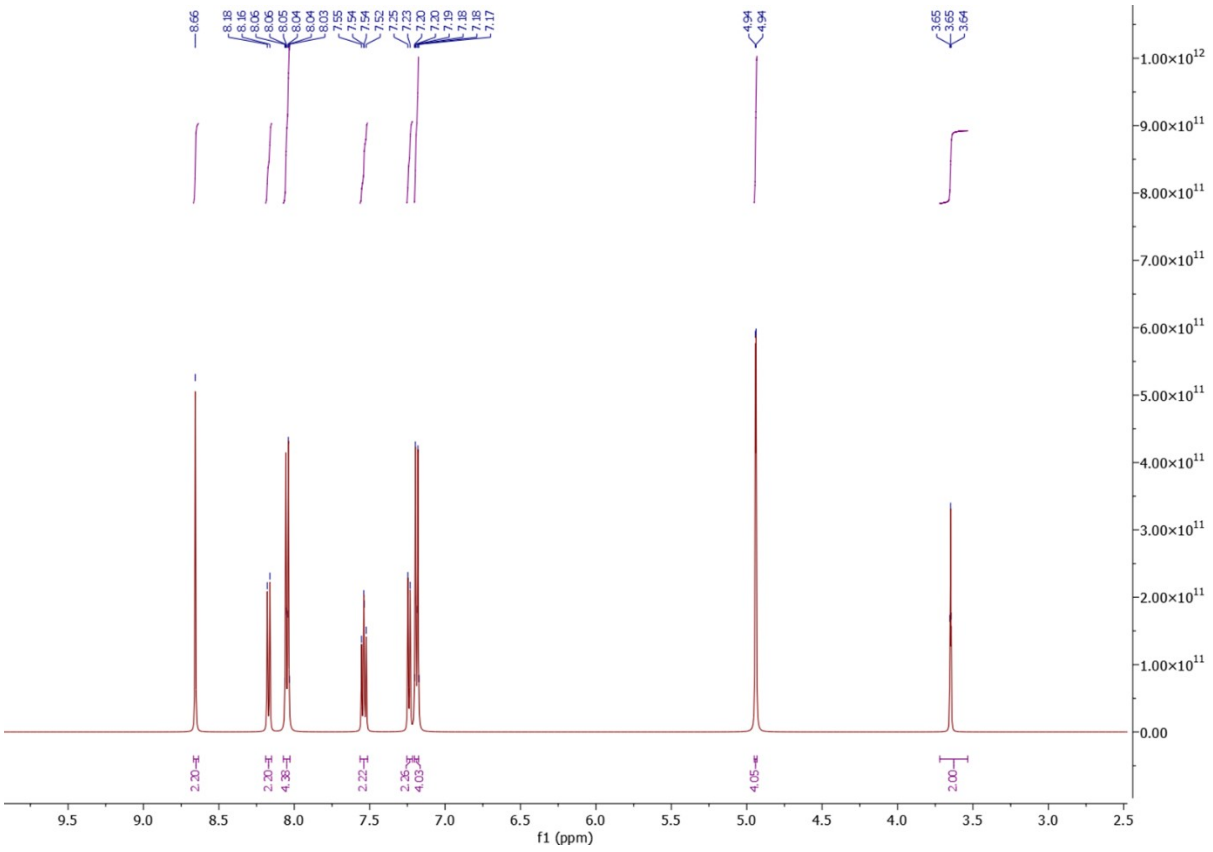

Figure S1: ^{1}H-NMR of compound 4

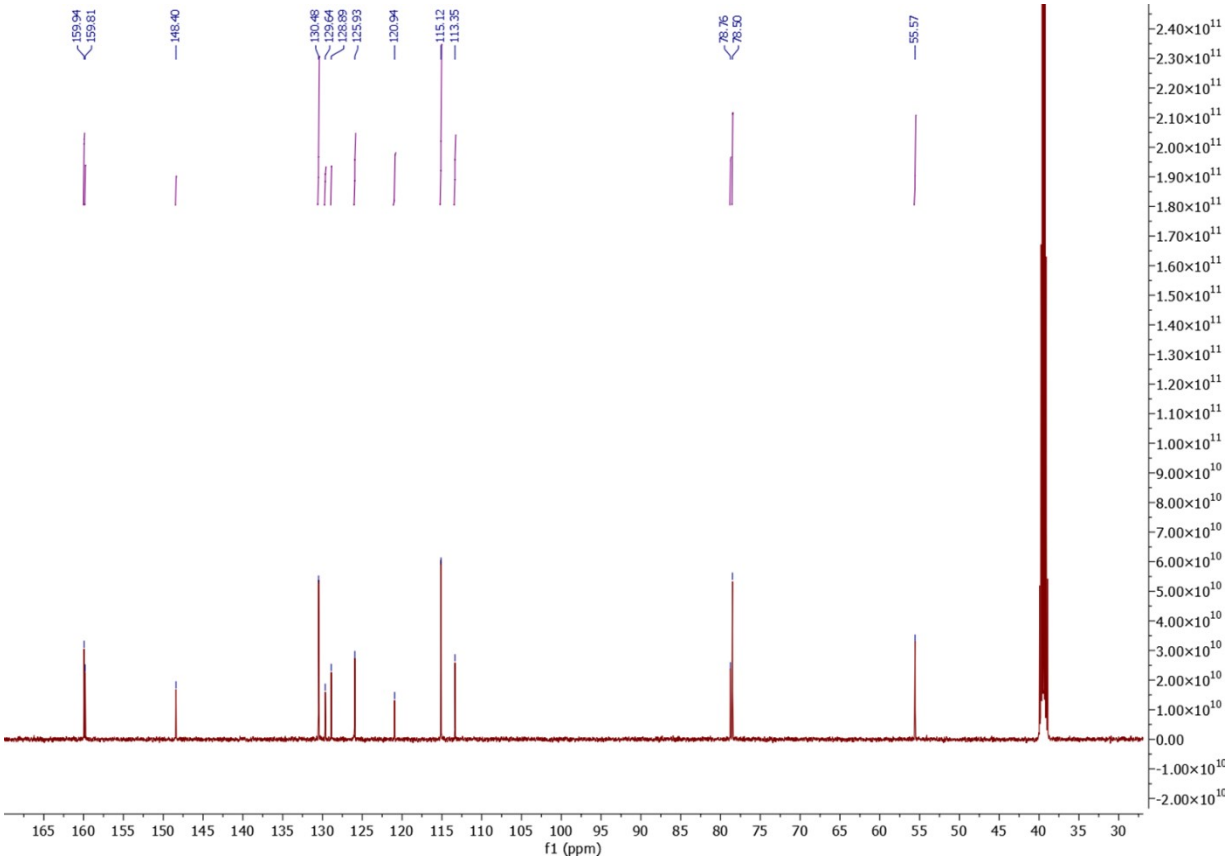

Figure S2: ^{13}C-NMR of compound 4

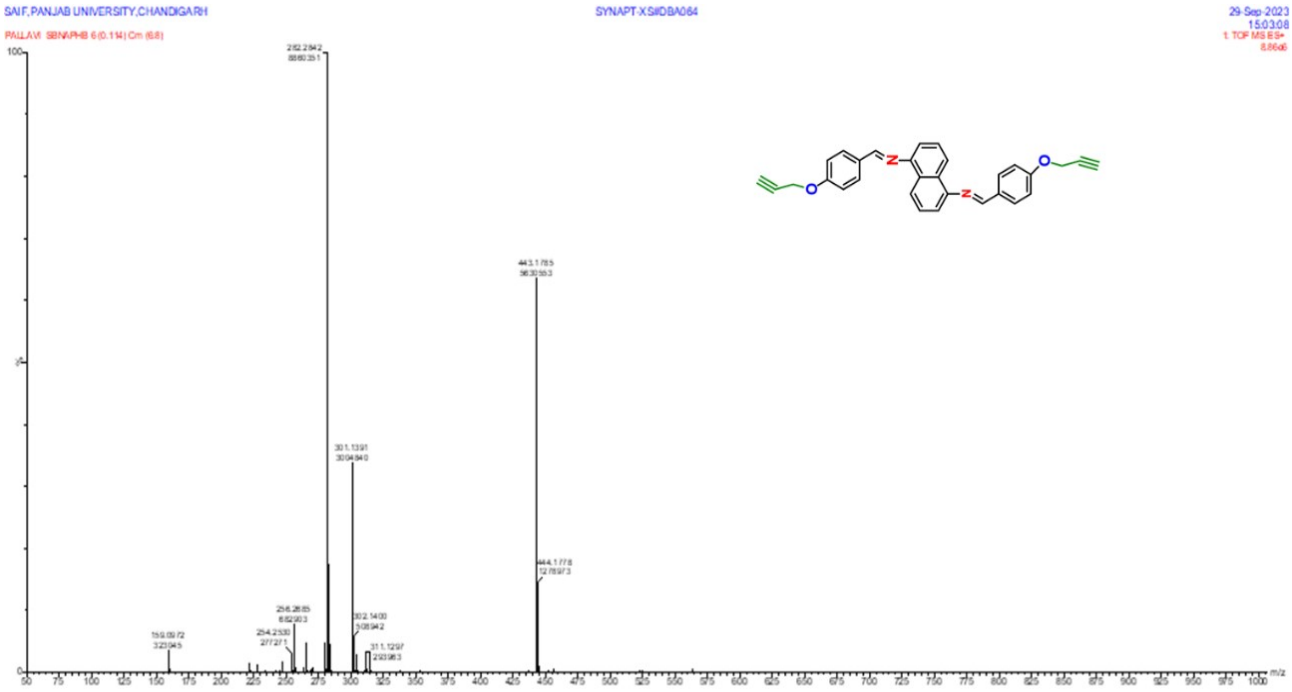

Figure S3: Mass Spectra of compound 4

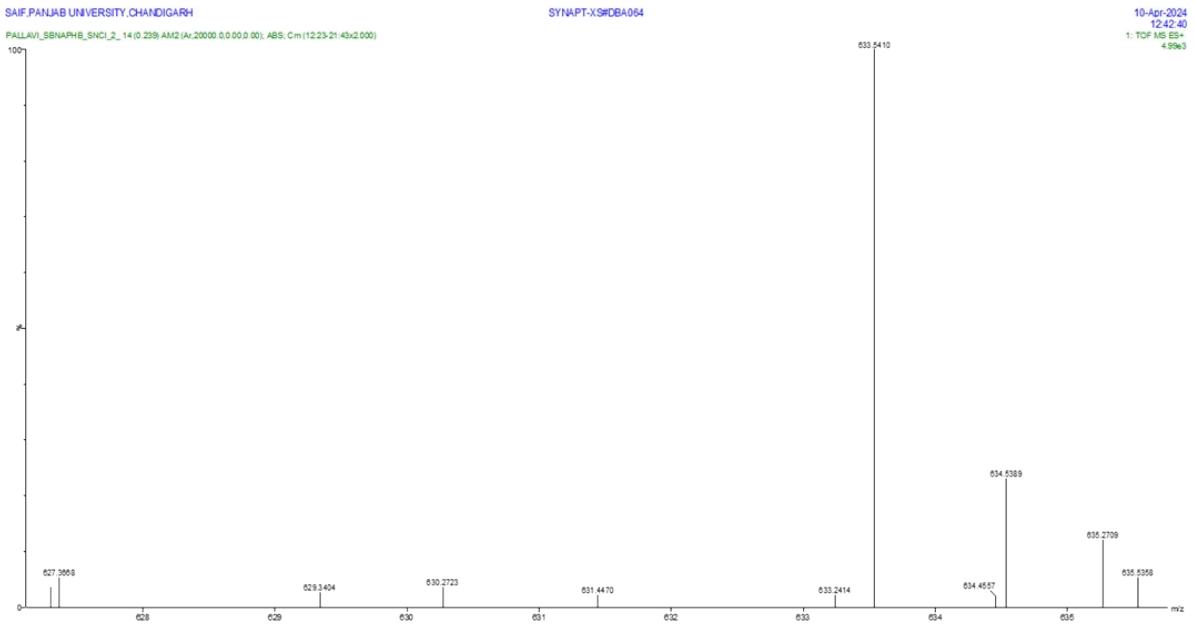

Figure S4 Mass Spectra of Metal complex

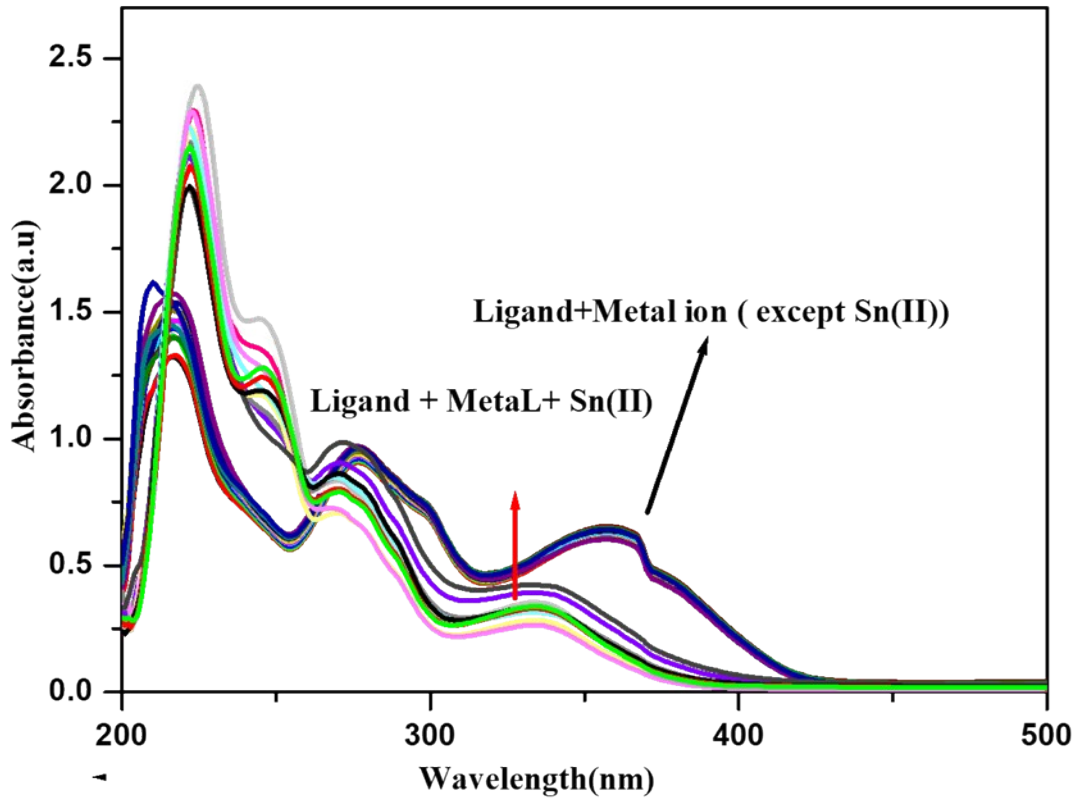

Fig. S 5 Anti interference studies

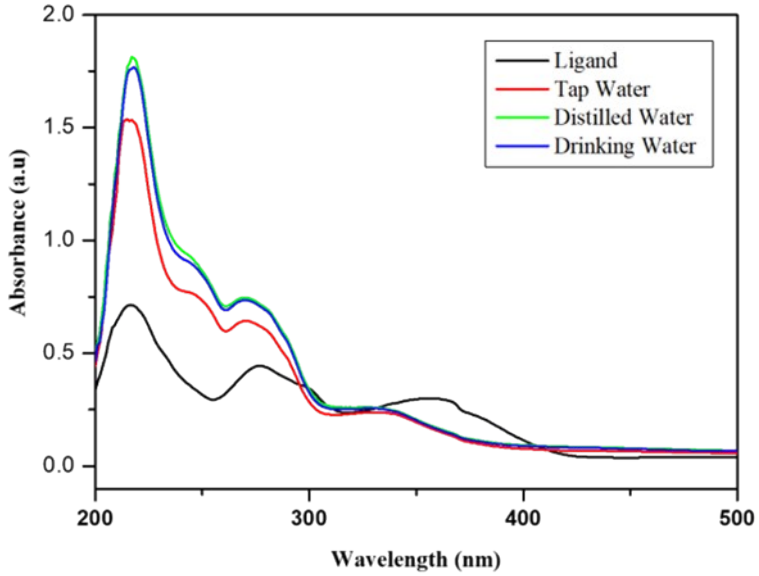

Fig S 6 Absorption spectra of Different water samples at 10^{-1}M of Sn(II)

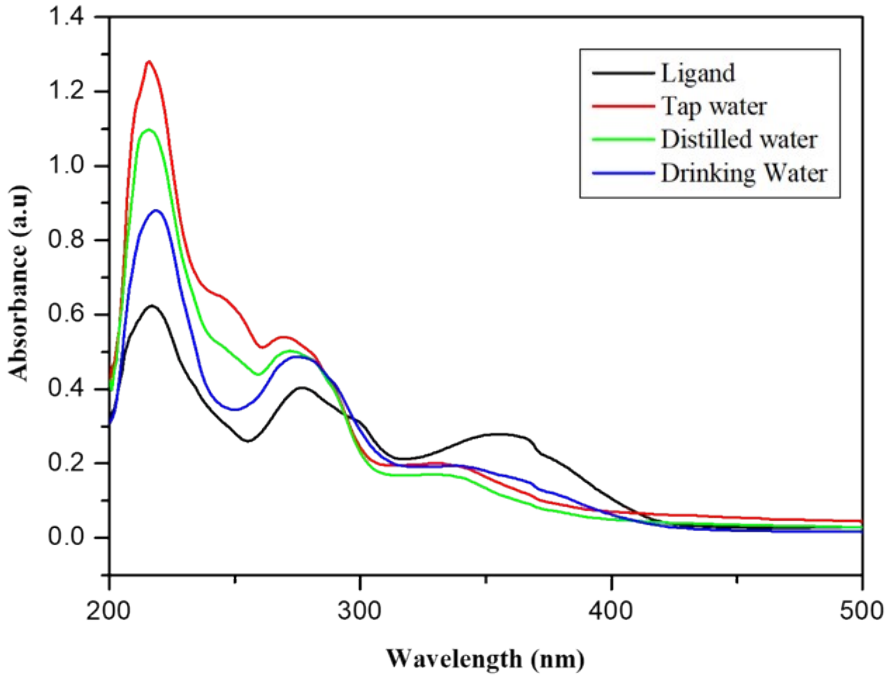

Fig S 7 Absorption spectra of Different water samples at 10^{-2}M of Sn(II).

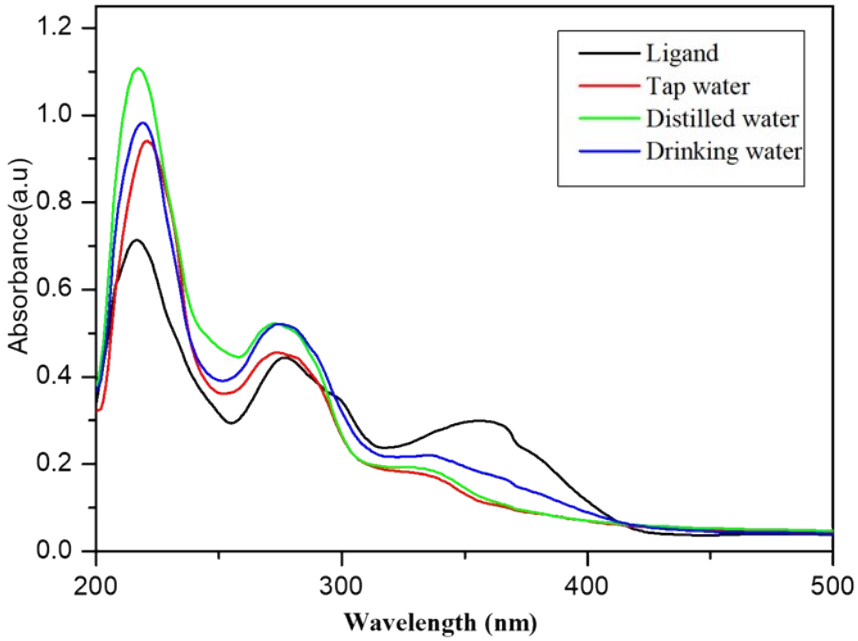

Fig S 8 Absorption spectra of Different water samples at 10^{-3}M of Sn(II).

Table S1 : Hydrophobic interactions

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	81A	THR	3.51	2872	764
2	111A	ALA	3.42	2864	1010
3	142A	LEU	3.04	2860	1279
4	189A	LEU	2.98	2882	1679
5	189A	LEU	2.82	2866	1677
6	212A	VAL	3.74	2883	1890
7	213A	PHE	2.87	2890	1900
8	250A	ILE	3.32	2890	2263

Table S2 Crystal data and structure refinement for compound 4

Identification code	try1
Empirical formula	$C_{15}H_{11}NO$
Formula weight	442.50
Temperature/K	293
Crystal system	triclinic
Space group	P-1
a/Å	7.8852(8)
b/Å	8.5306(7)
c/Å	9.6708(9)
α/°	85.411(7)
β/°	78.618(8)
γ/°	65.654(9)
Volume/Å^3	581.01(10)
Z	2
ρ_{calc}g/cm^3	1.265
μ/mm^{-1}	0.080
F(000)	232.1
Crystal size/mm^3	0.01 × 0.008 × 0.005
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.54 to 54.3
Index ranges	$-9 \le h \le 9$, $-9 \le k \le 10$, $-12 \le l \le 12$
Reflections collected	8330
Independent reflections	2417 [R_{int} = 0.0390, R_{sigma} = 0.0392]
Data/restraints/parameters	2417/0/154
Goodness-of-fit on F^2	0.965
Final R indexes [I>=2σ (I)]	R_1 = 0.0663, wR_2 = 0.2061
Final R indexes [all data]	R_1 = 0.0951, wR_2 = 0.2249
Largest diff. peak/hole / e Å^{-3}	0.25/-0.24

Table S3 Fractional Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for compound 4

Atom	*x*	*y*	*z*	U(eq)
O1	1990(3)	10424(3)	9641(2)	79.0(7)
N1	7893(4)	3619(3)	6284(2)	60.5(6)
C7	9133(4)	2384(3)	5241(3)	54.5(7)
C11	10629(4)	-637(3)	4500(3)	52.1(7)
C10	11624(4)	-157(4)	3274(3)	60.4(7)
C2	3236(4)	9422(4)	7208(3)	64.3(8)
C9	11384(4)	1505(4)	3071(3)	66.5(8)
C008	6843(4)	5081(4)	5886(3)	60.8(7)
C4	5586(4)	6490(3)	6850(3)	57.5(7)
C1	3155(4)	9211(4)	8646(3)	61.8(8)
C6	4306(5)	7661(4)	9187(3)	68.0(8)
C8	10143(4)	2779(4)	4055(3)	62.7(8)
C3	4442(4)	8053(4)	6327(3)	63.3(8)
C5	5518(4)	6322(4)	8302(3)	63.6(8)
C13	1703(5)	13159(4)	8636(3)	76.7(9)
C12	731(5)	12057(4)	9186(4)	76.7(9)
C14	2462(7)	14054(6)	8226(4)	102.3(13)

Table S4 Anisotropic Displacement Parameters ($Å^2 x\ 10^3$) for compound 4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U_{11} + 2\ h\ k\ a^*\ b^*\ U_{12+....}]$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	83.7(15)	64.3(13)	66.8(13)	-14.3(11)	1.2(11)	-1.8(10)
N1	65.5(15)	54.6(13)	61.1(14)	-24.4(12)	-7.9(12)	-6.1(11)
C7	56.0(16)	53.9(15)	56.7(15)	-23.4(13)	-13.3(13)	-2.9(12)
C11	52.2(15)	57.4(15)	51.7(14)	-24.8(12)	-13.8(12)	-2.2(11)
C10	61.5(17)	64.6(17)	56.8(16)	-28.7(14)	-4.5(13)	-7.0(13)
C2	58.9(17)	62.0(17)	65.9(18)	-15.9(14)	-18.1(14)	3.0(14)
C9	72(2)	71.1(19)	61.8(17)	-38.5(16)	-3.1(15)	1.0(14)
C008	61.2(17)	64.4(18)	59.5(17)	-27.6(15)	-10.1(14)	-5.1(14)
C4	58.9(17)	56.1(16)	61.6(16)	-27.2(13)	-10.7(13)	-1.3(13)
C1	59.3(17)	57.3(16)	63.8(18)	-22.3(14)	-1.9(14)	-3.4(14)
C6	82(2)	61.9(18)	53.7(16)	-26.6(16)	-6.3(15)	8.7(14)
C8	70.5(19)	58.5(16)	64.2(17)	-32.1(15)	-10.5(15)	1.0(13)
C3	65.5(18)	68.0(18)	55.7(16)	-23.5(15)	-19.0(14)	3.8(14)
C5	70.4(19)	55.6(16)	59.9(17)	-23.0(15)	-8.5(14)	4.8(13)
C13	86(2)	67(2)	73(2)	-24.6(19)	-22.7(18)	3.1(17)
C12	64(2)	64.8(19)	86(2)	-13.4(16)	-6.4(17)	-4.5(16)
C14	131(4)	107(3)	91(3)	-67(3)	-34(3)	17(2)

Table S5 Bond Lengths for Compound 4.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.367(3)	C2	C3	1.385(4)
O1	C12	1.433(4)	C9	C8	1.402(4)
N1	C7	1.420(3)	C008	C4	1.459(4)
N1	C008	1.260(4)	C4	C3	1.388(4)
C7	C11[1]	1.431(4)	C4	C5	1.392(4)
C7	C8	1.364(4)	C1	C6	1.390(4)
C11	C11[1]	1.415(5)	C6	C5	1.373(4)
C11	C10	1.417(4)	C13	C12	1.452(5)
C10	C9	1.354(4)	C13	C14	1.154(5)
C2	C1	1.379(4)			

[1]2-X,-Y,1-Z

Table S6 Bond Angles for Compound 4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C12	O1	C1	118.7(2)	C5	C4	C008	121.5(3)
C008	N1	C7	118.4(2)	C5	C4	C3	118.4(3)
C11[1]	C7	N1	117.2(2)	C2	C1	O1	125.3(3)
C8	C7	N1	123.2(2)	C6	C1	O1	114.6(3)
C8	C7	C11[1]	119.6(2)	C6	C1	C2	120.1(3)
C11[1]	C11	C7[1]	118.8(3)	C5	C6	C1	120.5(3)
C10	C11	C7[1]	121.7(2)	C9	C8	C7	121.1(3)
C9	C10	C11	120.2(3)	C4	C3	C2	121.8(3)
C3	C2	C1	118.8(3)	C6	C5	C4	120.3(3)
C8	C9	C10	120.9(3)	C14	C13	C12	178.5(4)
C4	C008	N1	123.7(3)	C13	C12	O1	112.1(3)
C3	C4	C008	120.1(3)				

[1]2-X,-Y,1-Z

Table S7 Torsion Angles for Compound 4.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C1	C2	C3	-177.7(3)	C7[1]	C11	C10	C9	-179.1(3)
O1	C1	C6	C5	178.8(3)	C7	C8	C9	C10	-0.4(4)
N1	C7	C11[1]	C11	-178.5(3)	C11[1]	C11	C10	C9	0.7(4)
N1	C7	C11[1]	C10[1]	1.7(3)	C11	C10	C9	C8	-0.6(3)
N1	C7	C8	C9	178.5(3)	C2	C1	C6	C5	-0.7(4)
N1	C008	C4	C3	-178.6(3)	C2	C3	C4	C008	-179.8(3)
N1	C008	C4	C5	2.4(4)	C2	C3	C4	C5	-0.7(3)
C7	C11[1]	C11	C7[1]	-180.0(3)	C008	C4	C5	C6	-179.2(3)
C7	C11[1]	C11	C10	0.2(3)	C4	C5	C6	C1	-1.1(4)

[1]2-X,-Y,1-Z