Supplementary Information

Weakly antiferromagnetic vanillin and acetate bridged dinuclear Ni(II) compound exhibiting catecholase-like activity and biological properties

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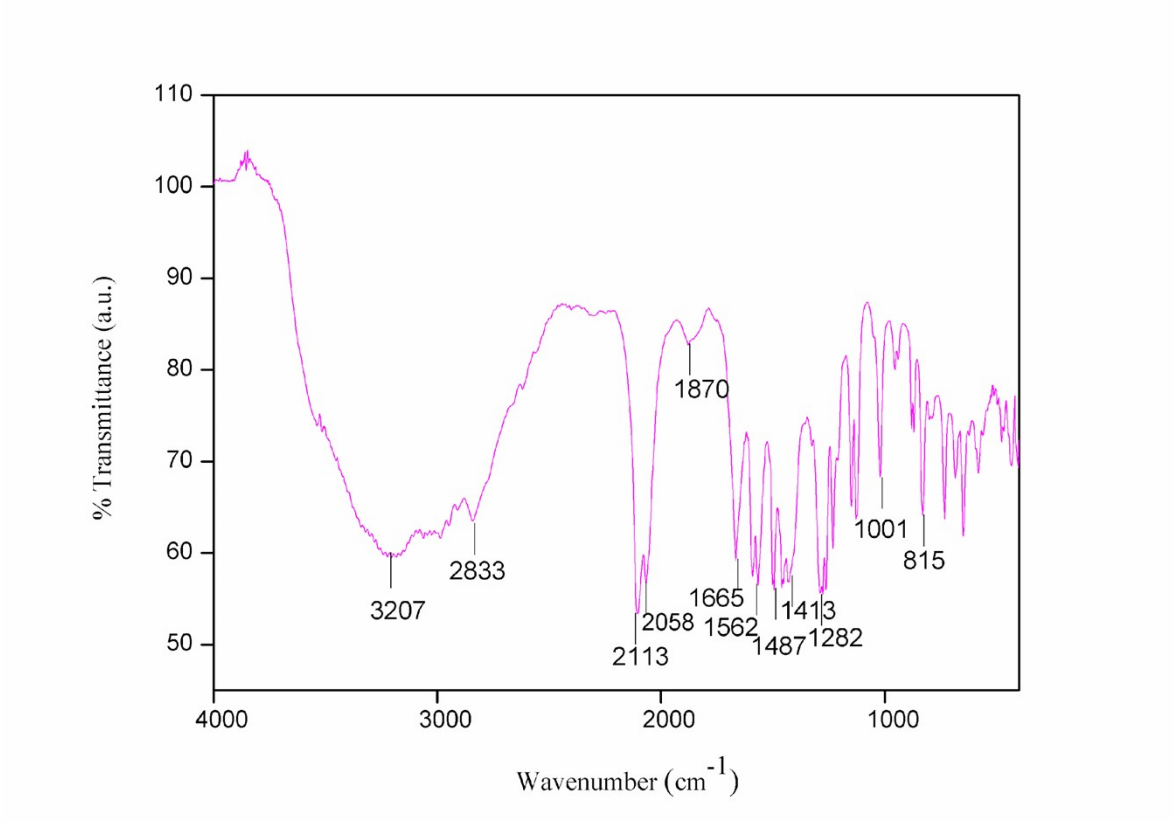

Fig. S1. Infrared spectrum of **1** recorded between 4000- 400 cm^{-1} at a resolution of 4 cm^{-1}.

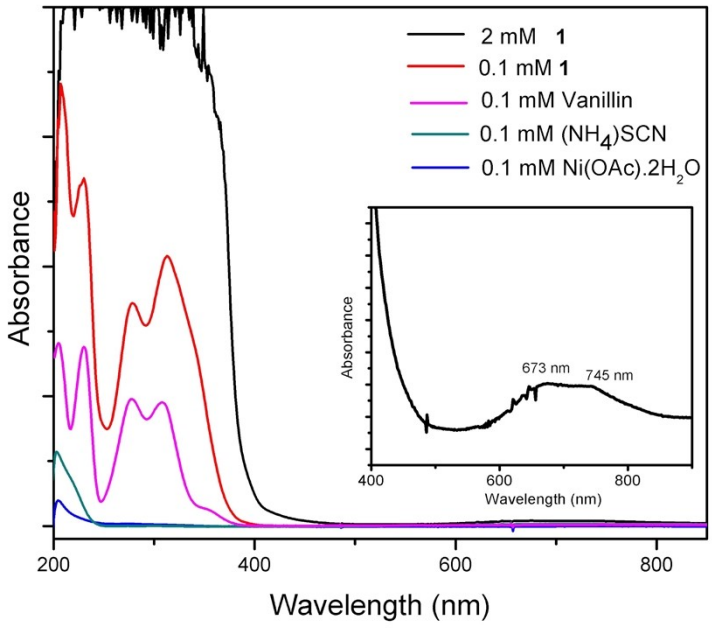

Fig. S2. UV-vis spectra of **1** and starting components recorded in MeOH

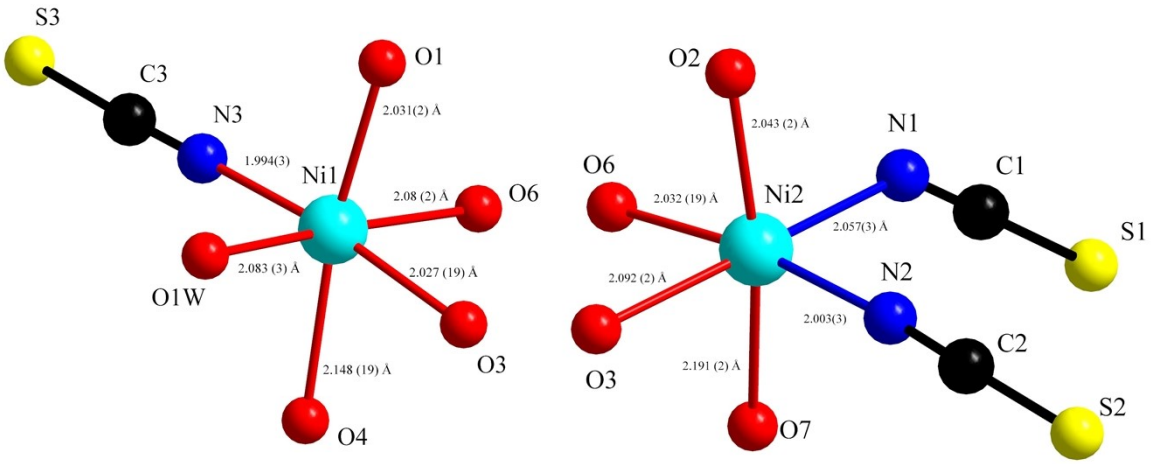

Fig. S3. The distorted octahedral geometry adopted by the Ni1 **(Left)** and Ni2 **(Right)** in the dinuclear compound.

Table S1. Selected bond length (Å) and angle (°) for compound **1**.

Ni1-O1	2.031(2)	Ni2-O2	2.043(2)
Ni1-O3	2.027(19)	Ni2-O3	2.092(2)
Ni1-O4	2.148(19)	Ni2-O6	2.032(18)
Ni1-O6	2.080(2)	Ni2-O7	2.191(2)
Ni1-N3	1.994(3)	Ni1-N1	2.057(3)
Ni1-O1W	2.083(3)	Ni1-N2	2.003(3)
N3-Ni1-O3	171.81(9)	N2-Ni2-O2	94.10(11)
N3-Ni1-O1	95.87(10)	O6-Ni2-O2	93.06(8)
O3-Ni1-O1	92.13(8)	N2-Ni2-N1	92.23(13)
N3-Ni1-O6	94.66(10)	O6-Ni2-N1	91.72(11)
O3-Ni1-O6	83.61(8)	O2-Ni2-N1	93.58(11)
O1-Ni1-O6	89.64(9)	N2-Ni2-O3	92.49(10)
N3-Ni1-O1W	92.64(12)	O6-Ni2-O3	83.17(8)
O3-Ni1-O1W	89.31(11)	O2-Ni2-O3	89.43(8)
O1-Ni1-O1W	88.53(12)	N1-Ni2-O3	174.21(10)
O6-Ni1-O1W	172.62(10)	N2-Ni2-O7	96.27(10)
N3-Ni1-O4	94.91(9)	O6-Ni2-O7	76.48(7)
O3-Ni1-O4	77.11(7)	O2-Ni2-O7	169.50(8)
O1-Ni1-O4	169.18(8)	N1-Ni2-O7	87.68(11)
O6-Ni1-O4	90.34(8)	O3-Ni2-O7	88.47(7)

O1W-Ni1-O4	90.12(12)	N2-Ni2-O6	171.59(10)
Ni1-O3-Ni2	93.52(8)	Ni1-O6-Ni2	93.73(8)

Table S2. The geometric parameters of the Isothiocyanate, acetate and *p*-vanillin ligands

Bond distance (Å) and angle (°)			
Isothiocyanate			
S1-C1	1.626(4)	N1-C1-S1	179.6(4)
S2-C2	1.626(3)	N2-C2-S2	178.3(4)
S3-C3	1.634(3)	N3-C3-S3	178.1(4)
Acetate			
O1-C4	1.254(4)	O1-C4-O2	125.0(3)
O2-C4	1.254(4)	O1-C4-C5	117.4(3)
C4-C5	1.519(5)	O2-C4-C5	117.6(3)
***p*-Vanillin**			
O3-C6	1.342(3)	O3-C6-C7	122.8(2)
C6-C7	1.386(4)	O3-C6-C11	118.7(2)
C7-C8	1.384(4)	C7-C6-C11	118.5(3)
C8-C9	1.385(5)	C8-C7-C6	120.2(3)
C9-C10	1.404(4)	C9-C8-C7	120.6(3)
C10-C11	1.365(4)	C8-C9-C10	120.1(3)
C6-C11	1.414(4)	C8-C9-C13	120.3(3)
C9-C13	1.458(5)	C10-C9-C13	119.6(3)
O5-C13	1.209(5)	C11-C10-C9	118.9(3)
O4-C11	1.377(3)	C10-C11-O4	125.1(2)
O4-C12	1.433(3)	C10-C11-C6	121.7(2)
O6-C14	1.343(3)	O4-C11-C6	113.3(2)
C14-C15	1.419(4)	O5-C13-C9	125.0(3)
C15-C16	1.373(4)	O6-C14-C19	122.5(2)
C16-C17	1.402(4)	O6-C14-C15	118.9(2)
C17-C18	1.395(4)	C19-C14-C15	118.5(3)
C18-C19	1.379(4)	C16-C15-O7	125.4(2)
C14-C19	1.388(4)	C16-C15-C14	121.3(3)
O7-C15	1.380(3)	O7-C15-C14	113.3(2)
O7-C20	1.432(3)	C15-C16-C17	119.2(3)
C17-C21	1.453(4)	C18-C17-C16	119.8(3)
O8-C21	1.214(4)	C18-C17-C21	118.8(3)
		C16-C17-C21	121.4(3)
		C19-C18-C17	120.7(3)
		C18-C19-C14	120.5(3)
		O8-C21-C17	126.2(4)

Comment [nh]: Original:Thiocyanate New: Isothiocynate

Comment [nh]: Original: Vanilate new: vanillin

Comment [nh]: Original: vanilate New: vanillin

Table S3. The hydrogen bonding parameters of **1**.

D-H···A	d(D-H)	d(H···A)	<DHA	d(D···A)	Symmetry code
O1W-H1A···S1	0.883	2.408	171.04	3.283	[x-1, y, z]
O1W-H1B···O5W	0.714	2.142	168.29	2.845	[x-1, y-1/2, z-3/2]
C5-H5A···O8	0.96	2.621	157.18	3.526	[x-1, y-1/2, z-3/2]
C13-H13···S1	0.93	2.937	172.06	3.86	[x-1, y-1, z-2]

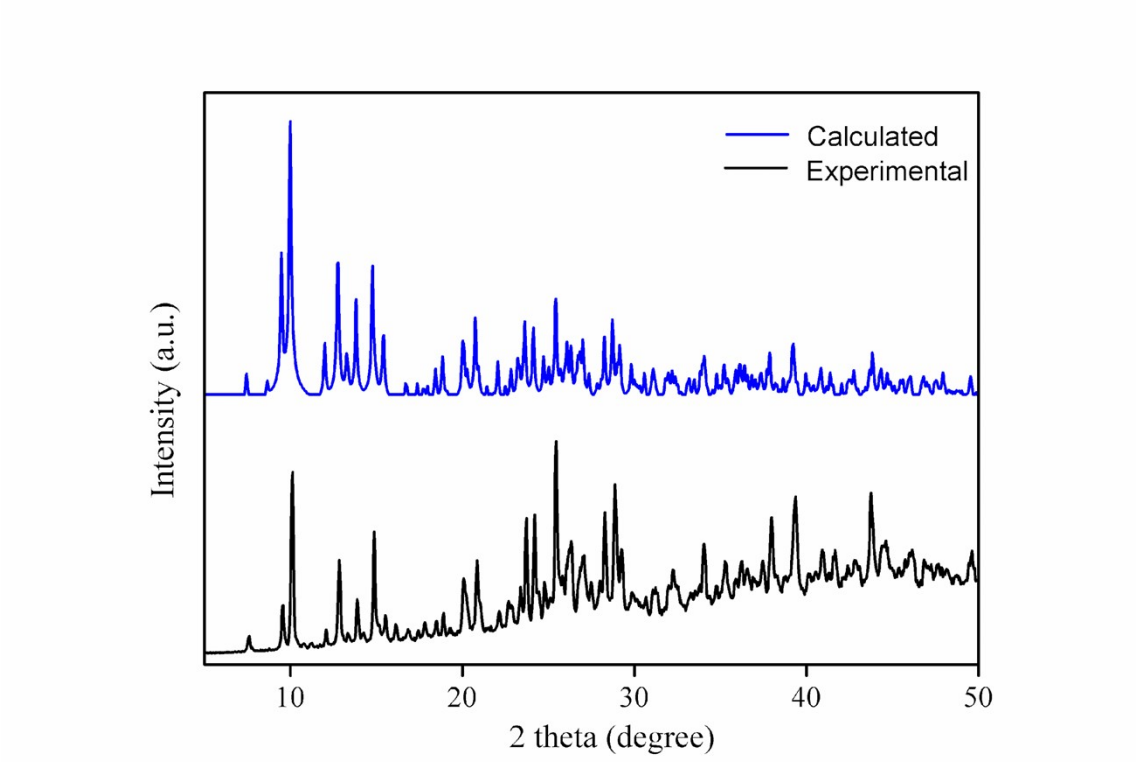

Fig. S4. Comparison of experimental (black) and simulated (blue) PXRD patterns of compound**1**

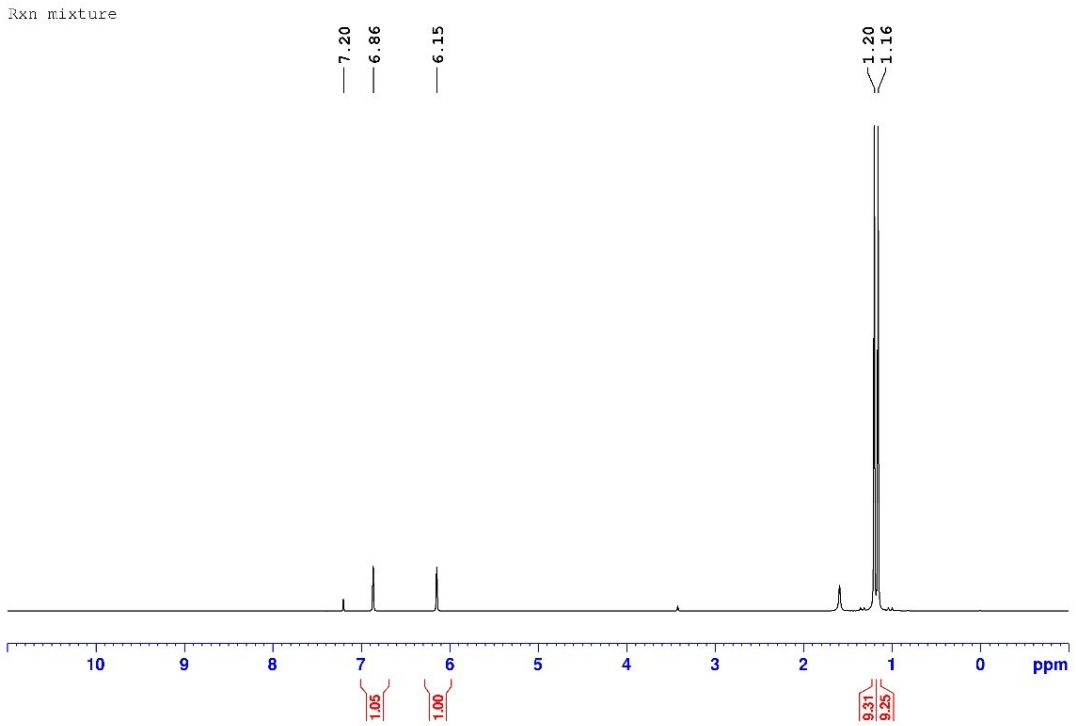

Fig. S5. ^{1}H NMR of the product obtained after the catalytic reaction.

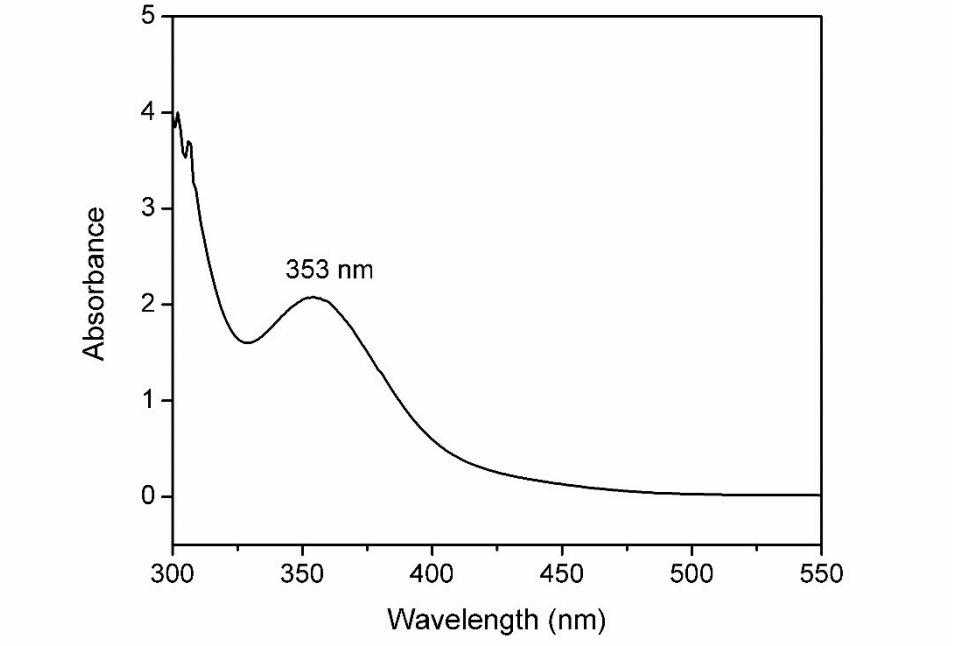

Fig. S6. Detection of H_2O_2 using UV-Vis spectra showing a characteristic peak of I^{3-} after DTBC oxidation with compound **1** (10^{-4}M)

Table S4. Kinetic data for catecholase activity of mono- and dinuclear nickel compounds

Sr.No	Catalyst	Solvent	Kcat(h^{-1})	Ref.
1	$[NiL^2(H_2O)_3](NO_3)_2$	methanol	52.6 x 10^1	S1
2	$[NiL^1(H_2O)_3]I_2{\cdot}H_2O$	methanol	92.7	S2
3	$[Ni_2(L^1)_2(CH_3CN)_4](ClO_4)_2{\cdot}2CH_3CN$	methanol	7.9	S3
4	$[Ni_2L_2(PhCOO)(H_2O)_2]ClO_4$	methanol	167.6	S4
5	$[NiL(H_2O)_3](NO_3)_2$	methanol	1500	S5
6	$[Ni_2(L^2)(SCN)_3(H_2O)(CH_3OH)]$	methanol	154.6	S6
7	$[Mn(HL)_2]{\cdot}2ClO_4$	methanol	1038	S7
8	$[Cu(L^1H^{py})Cl]_2(ClO_4)_2$	methanol	$3.46x10^5$	S8
9	$[Ni_2(\mu\text{-van})_2(\mu\text{-OAc})(NCS)_3(H_2O)]{\cdot}5H_2O$	methanol	157.1 $x10^2$	This work

Abbreviations: L^2 **(1)** = N-(2-aminoethyl)piperazine, HL^1 **(2)** = 2-[(2-piperazin-1-ylethylimino)-methyl]phenol], HL^1 **(3)** = 2-[(3-methylamino-propylamino)-methyl]-4-phenol], HL_2 **(4)** = [(3-dimethylamino-propylamino)-methyl]-phenol, H_2L **(5)** = N,N'-propylene-bis(3-formyl-5-tert-butylsalicylaldimine), μ-van **(6)** = *p*-vanillin, L^2 **(7)** = 2,6-bis(N,N-dimethyl ethylene-iminomethyl)-4-methyl-phenolato,

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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) nvscn_0m

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No syntax errors found. CIF dictionary Interpreting this report

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Bond precision:   C-C = 0.0042 A          Wavelength=0.71073

Cell:             a=10.6374(14)     b=22.981(3)         c=14.4274(17)
                  alpha=90          beta=106.458(4)     gamma=90
Temperature:      296 K
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Hall group	-P 2ybc	-P 2ybc
Moiety formula	C21 H21 N3 Ni2 O9 S3, 5(H2 O)	C21 H21 N3 Ni2 O9 S3, 5(H2 O)
Sum formula	C21 H31 N3 Ni2 O14 S3	C21 H31 N3 Ni2 O14 S3
Mr	763.05	763.09
Dx,g cm-3	1.498	1.498
Z	4	4
Mu (mm-1)	1.361	1.361
F000	1576.0	1576.0
F000'	1580.92	
h,k,lmax	14,30,19	14,30,19
Nref	8471	8412
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Tmin'	0.574	

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test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

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PLAT420_ALERT_2_B D-H Bond Without Acceptor  O5W       --H5WB      .     Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor  O6W       --H6WB      .     Please Check
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Alert level C

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PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O5W      0.134 Check
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PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         14 Report
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             -11  7  9, -11  5 10,
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Alert level G

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              H6WB
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