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4-(1*H*-1,2,4-三唑-1-亚甲基)苯甲酸过渡金属配合物的合成、结构、抑菌活性及 DNA 裂解活性

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Syntheses, Structures, Antifungal Activities and DNA Cleavage of Transition Metal Coordination Compounds with 4-(1*H*-1,2,4-triazol-1-ylmethyl) Benzoic Acid

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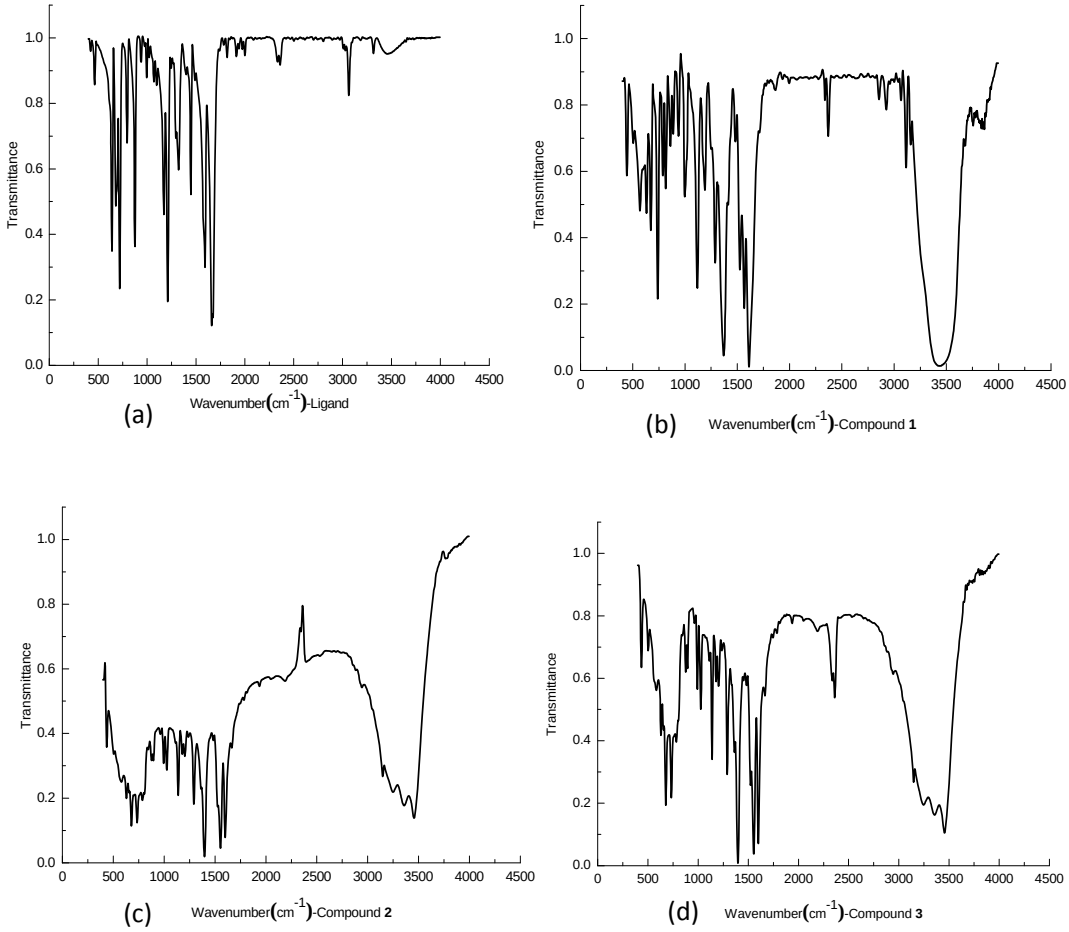

Fig.S1 The IR spectra of the ligand and compounds **1-3**

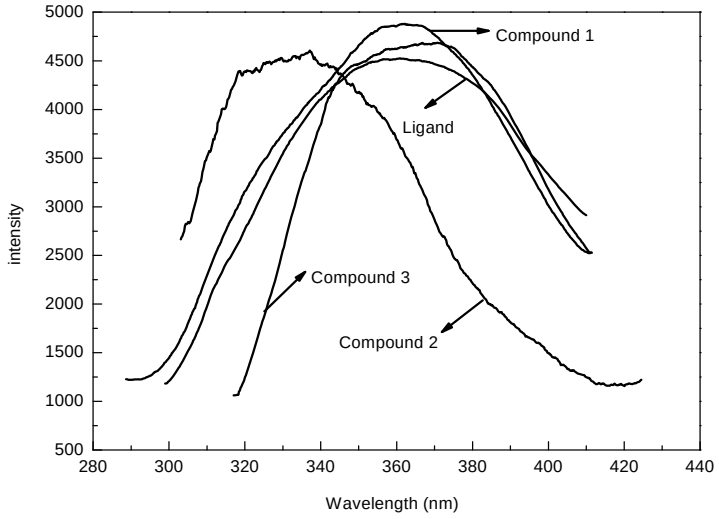

Fig.S2 Excitation spectra of the ligand and compounds in the solid state at room temperature

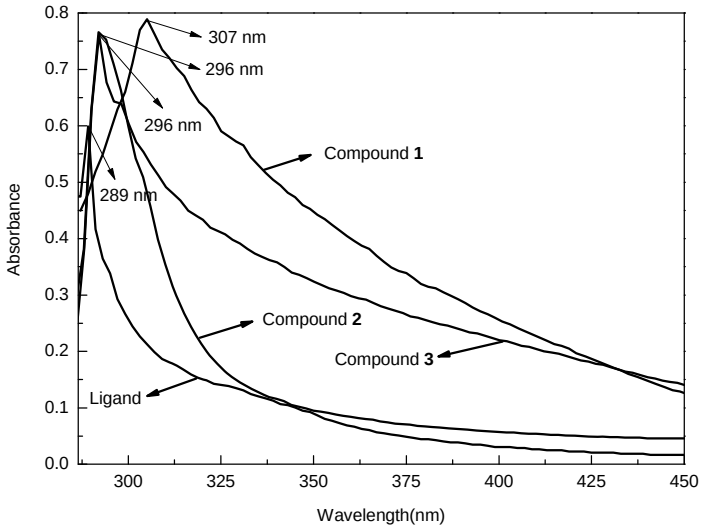

Fig.S3 UV-vis spectra of the ligand and compounds in dimethyl sulfoxide (DMSO) solvent at room temperature

Table S1 Selected bond lengths (nm) and angles (°) for metal environments of the compounds

Compound **1**				
	Cu(1)-O(1)	0.1949(5)	Cu(1)-O(2)	0.2739
	Cu(1)-N(3)	0.1986(5)	O(1)-Cu(1)-N(3)	90.4(2)
	O(1)#1-Cu(1)-O(1)	180.000(2)	O(1)#1-Cu(1)-N(3)	89.6(2)
Compound **2**				
	Ni(1)-O(1)	0.2050(2)	Ni(1)-N(1)	0.2063(3)
	Ni(1)-O(3)	0.2097(2)	O(1)-Ni(1)-O(1)#1	180.000(1)
	O(1)-Ni(1)-N(1)#1	90.85(10)	N(1)-Ni(1)-O(3)	93.16(10)
	O(1)-Ni(1)-N(1)	89.15(10)	N(1)#1-Ni(1)-N(1)	180.000(1)
	O(1)-Ni(1)-O(3)#1	86.19(9)	N(1)-Ni(1)-O(3)#1	86.84(10)
	O(1)-Ni(1)-O(3)	93.81(9)		
Compound **3**				
	Co(1)-O(1)	0.20702(13)	Co(1)-N(1)	0.21248(16)
	Co(1)-O(3)	0.21343(14)	N(1)-Co(1)-O(3)	93.20(6)
	O(1)-Co(1)-O(1)#1	180.0	O(1)-Co(1)-N(1)	89.32(6)
	O(1)-Co(1)-N(1)#1	90.68(6)	O(3)#1-Co(1)-O(3)	180.00(5)
	O(1)#1-Co(1)-N(1)#1	89.32(6)	N(1)-Co(1)-N(1)#1	180.0
	O(1)-Co(1)-O(3)#1	86.78(5)	N(1)-Co(1)-O(3)#1	86.80(6)
	O(1)-Co(1)-O(3)	93.22(5)		

Table S2 Virulence regression equations of three compounds against on five fungi

Fungi	Compounds	Virulence regression equation	EC50
Fusarium graminearum	**1**	$y = 4.8262x - 2.6772$ $R^2 = 0.9962$	38.97
	2	$y = 8.8383x - 12.933$ $R^2 = 0.9549$	106.908
	3	$y = 7.8923x - 11.273$ $R^2 = 0.9747$	115.3143
Colletotrichum gloeosporioides	**1**	$y = 6.3607x - 7.5575$ $R^2 = 0.9906$	93.33
	2	$y = 6.2166x - 8.1095$ $R^2 = 0.9205$	128.4663
	3	$y = 9.0059x - 14.012$ $R^2 = 0.9333$	129.1399
Vasa mali	**1**	$y = 6.8263x - 5.344$ $R^2 = 0.9993$	33.11
	2	$y = 11.627x - 16.045$ $R^2 = 0.9885$	64.56709
	3	$y = 6.774x - 5.4809$ $R^2 = 0.9997$	35.25532
Alternaria alternata	**1**	$y = 13.56x - 20.561$ $R^2 = 0.9965$	77.62
	2	$y = 13.736x - 21.058$ $R^2 = 0.9699$	78.8967
	3	$y = 14.061x - 21.828$ $R^2 = 0.9956$	80.90445
Macrophoma kawatsukai	**1**	$y = 9.1563x - 12.461$ $R^2 = 0.9846$	81.28
	2	$y = 9.3872x - 14.767$ $R^2 = 0.9917$	127.5674
	3	$y = 9.1047x - 13.587$ $R^2 = 0.9631$	110.0204