Electronic Supplementary Information

Solvent effect on the structures of three manganese complexes based on azotetrazolyl-3-hydroxy-2-naphthoic acid: syntheses, structures, magnetic and fluorescent properties

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Contents of the Electronic Supplementary Information

Table S1 Selected bond lengths [Å] and angles [°] for complex **1**.

Bond distances			
Mn(1)–N(1)	2.085(2)	Mn(1)–N(2)	2.103(2)
Mn(1)–N(3a)	2.100(2)	Mn(1)–O(1)	2.0554(18)
Mn(1)–O(2)	2.0881(17)	Mn(1)–O(3)	2.1397(19)
Angles			
N(1)-Mn(1)-N(2)	75.45(8)	N(1)-Mn(1)-N(3a)	100.47(8)
N(1)-Mn(1)-O(1)	153.53(8)	N(1)-Mn(1)-O(2)	92.32(8)
N(1)-Mn(1)-O(3)	92.20(8)	N(2)-Mn(1)-N(3a)	175.81(8)
N(2)-Mn(1)-O(1)	78.20(8)	N(2)-Mn(1)-O(2)	88.02(8)
N(2)-Mn(1)-O(3)	88.10(8)	N(3a)-Mn(1)-O(1)	105.91(8)
N(3a)-Mn(1)-O(2)	91.18(8)	N(3i)-Mn(1)-O(3)	93.10(8)
O(1)-Mn(1)-O(2)	89.34(7)	O(1)-Mn(1)-O(3)	84.31(7)
O(2)-Mn(1)-O(3)	173.12(7)		

[a] 1-x, 1-y, -z

Table S2 Selected bond lengths [Å] and angles [°] for complex **2**.

Bond distances			
Mn(1)–N(1)	2.311(3)	Mn(1)–N(2)	2.430(3)
Mn(1)–O(1)	2.230(3)	Mn(1)–O(1a)	2.252(2)
Mn(1)–O(2)	2.181(3)	Mn(1)–O(3)	2.161(3)
Mn(1)–O(4a)	2.242(2)	Mn(2)–N(3)	2.153(3)
Mn(2)–N(3c)	2.153(3)	Mn(2)–O(4a)	2.241(2)
Mn(2)–O(4b)	2.241(2)	Mn(2)–O(5a)	2.199(3)
Mn(2)–O(5b)	2.199(3)		
Angles			
N(1)-Mn(1)-N(2)	65.35(10)	N(1)-Mn(1)-O(1a)	147.89(10)
N(1)-Mn(1)-O(1)	132.96(10)	N(1)-Mn(1)-O(2)	88.68(11)

N(1)-Mn(1)-O(3)	93.24(13)	N(1)-Mn(1)-O(4a)	146.41(10)
N(2)-Mn(1)-O(1)	67.96(9)	N(2)-Mn(1)-O(1a)	86.71(9)
N(2)-Mn(1)-O(2)	91.49(11)	N(2)-Mn(1)-O(3)	86.11(12)
N(2)-Mn(1)-O(4a)	137.40(10)	O(1)-Mn(1)-O(1a)	79.15(9)
O(1)-Mn(1)-O(2)	87.09(10)	O(1)-Mn(1)-O(3)	89.02(12)
O(1)-Mn(1)-O(4a)	154.61(9)	O(1a)-Mn(1)-O(2)	93.55(10)
O(1a)-Mn(1)-O(3)	86.70(12)	O(1a)-Mn(1)-O(4a)	75.80(9)
O(2)-Mn(1)-O(3)	175.98(12)	O(2)-Mn(1)-O(4a)	90.38(10)
O(3)-Mn(1)-O(4a)	93.57(12)	N(3)-Mn(2)-N(3c)	91.50(19)
N(3)-Mn(2)-O(4a)	82.09(11)	N(3)-Mn(2)-O(4b)	123.83(11)
N(3)-Mn(2)-O(5a)	138.87(11)	N(3)-Mn(2)-O(5b)	99.64(12)
N(3c)-Mn(2)-O(4a)	123.83(11)	N(3c)-Mn(2)-O(4b)	82.09(11)
N(3c)-Mn(2)-O(5a)	99.64(12)	N(3c)-Mn(2)-O(5b)	138.87(11)
O(4a)-Mn(2)-O(4b)	145.05(14)	O(4a)-Mn(2)-O(5a)	58.81(9)
O(4a)-Mn(2)-O(5b)	96.99(10)	O(4b)-Mn(2)-O(5a)	96.99(10)
O(4b)-Mn(2)-O(5b)	58.81(9)	O(5a)-Mn(2)-O(5b)	97.44(16)

[a]1/2-x, 1/2-y, 1-z; [b]1/2+x, 1/2-y, 1/2+z; [c]1-x, +y, 3/2-z

Table S3 Selected bond lengths [Å] and angles [°] for complex **3**.

Bond distances			
Mn(1)–O(1)	2.292(3)	Mn(1)–O(2)	2.189(4)
Mn(1)–O(3)	2.183(4)	Mn(1)–O(4)	2.169(4)
Mn(1)–O(1b)	2.235(3)	Mn(1)–N(1b)	2.332(4)
Mn(1)–N(6b)	2.408(4)	Mn(2)–O(4)	2.443(4)
Mn(2)–O(5)	2.192(4)	Mn(2)–O(6)	2.293(4)
Mn(2)–O(7)	2.220(5)	Mn(2)–O(8)	2.315(3)
Mn(2)–N(2b)	2.278(5)	Mn(2)–N(8a)	2.283(5)
Mn(3)–O(8)	2.256(4)	Mn(3)–O(9)	2.195(3)
Mn(3)–O(9a)	2.243(4)	Mn(3)–O(10)	2.180(4)

Mn(3)–O(11)	2.204(4)	Mn(3)–N(7a)	2.280(4)
Mn(3)–N(12a)	2.407(4)		
Angles			
O(1)-Mn(1)-O(2)	93.17(15)	O(1)-Mn(1)-O(3)	95.34(15)
O(1)-Mn(1)-O(4)	77.41(13)	O(1)-Mn(1)-O(1b)	76.12 (14)
O(1)-Mn(1)-N(1b)	149.52(14)	O(1)-Mn(1)-N(6b)	144.55(14)
O(2)-Mn(1)-O(3)	171.46(16)	O(2)-Mn(1)-O(4)	88.07(17)
O(2)-Mn(1)-O(1b)	85.57(16)	O(2)-Mn(1)-N(1b)	85.57(16)
O(2)-Mn(1)-N(6b)	89.37(16)	O(3)-Mn(1)-O(4)	93.05(18)
O(3)-Mn(1)-O(1b)	91.87(15)	O(3)-Mn(1)-N(1b)	86.71(16)
O(3)-Mn(1)-N(6b)	84.13(16)	O(4)-Mn(1)-O(1b)	153.40(14)
O(4)-Mn(1)-N(1b)	72.12(15)	O(4)-Mn(1)-N(6b)	138.03(15)
O(1b)-Mn(1)-N(1b)	134.30(14)	O(1b)-Mn(1)-N(6b)	68.49(14)
N(1b)-Mn(1)-N(6b)	65.92(15)	O(4)-Mn(2)-O(5)	54.98(14)
O(4)-Mn(2)-O(6)	140.79(14)	O(4)-Mn(2)-O(7)	90.3(2)
O(4)-Mn(2)-O(8)	161.52(13)	O(4)-Mn(2)-N(2b)	76.64(14)
O(4)-Mn(2)-N(8a)	85.57(16)	O(5)-Mn(2)-O(6)	86.46(15)
O(5)-Mn(2)-O(7)	90.7(2)	O(5)-Mn(2)-O(8)	139.99(15)
O(5)-Mn(2)-N(2b)	131.40(15)	O(5)-Mn(2)-N(8a)	95.84(18)
O(6)-Mn(2)-O(7)	82.63(19)	O(6)-Mn(2)-O(8)	56.92(13)
O(6)-Mn(2)-N(2b)	140.14(16)	O(6)-Mn(2)-N(8a)	107.42(17)
O(7)-Mn(2)-O(8)	99.06(19)	O(7)-Mn(2)-N(2b)	84.70(19)
O(7)-Mn(2)-N(8a)	168.29(19)	O(8)-Mn(2)-N(2b)	88.31(14)
O(8)-Mn(2)-N(8a)	82.13(14)	N(2b)-Mn(2)-N(8a)	83.69(17)
O(8)-Mn(3)-O(9)	78.48(13)	O(8)-Mn(3)-O(9a)	149.33(13)
O(8)-Mn(3)-O(10)	80.86(14)	O(8)-Mn(3)-O(11)	91.76(15)
O(8)-Mn(3)-N(7a)	75.87(14)	O(8)-Mn(3)-N(12a)	140.04(13)
O(9)-Mn(3)-O(9a)	73.96(14)	O(9)-Mn(3)-O(10)	99.16(15)
O(9)-Mn(3)-O(11)	84.18(16)	O(9)-Mn(3)-N(7a)	150.34(15)

O(9)-Mn(3)-N(12a)	141.19(15)	O(9a)-Mn(3)-O(10)	90.41(15)
O(9a)-Mn(3)-O(11)	98.50(16)	O(9a)-Mn(3)-N(7a)	150.34(15)
O(9a)-Mn(3)-N(12a)	67.56(13)	O(10)-Mn(3)-O(11)	171.06(16)
O(10)-Mn(3)-N(7a)	91.26(15)	O(10)-Mn(3)-N(12a)	86.24(15)
O(11)-Mn(3)-N(7a)	81.98(16)	O(11)-Mn(3)-N(12a)	96.38(16)
N(7a)-Mn(3)-N(12a)	66.73(15)		

[a]1-x, 1-y, -z; [b]1-x, -y, 1-z

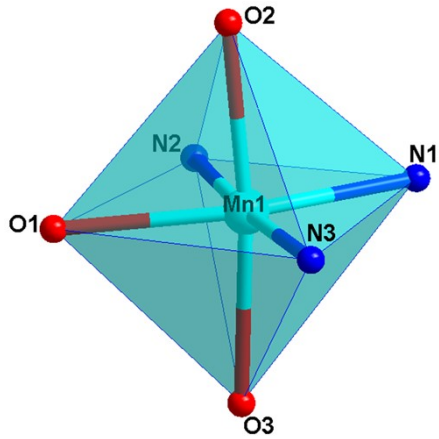

Figure S1 Local coordination geometry of Mn(II) ion in complex **1**.

Table S4 SHAPE analysis for complex **1**.

Complex	**M**	PPY-6	**OC-6**	TPR-6	JPPY-6
1	**Mn1**	20.007	**1.282**	12.881	28.716

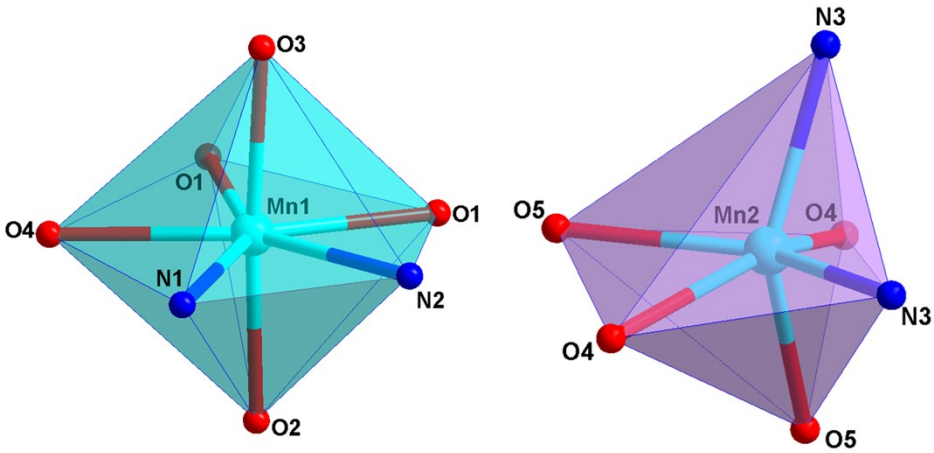

Figure S2 Local coordination geometry of Mn(II) ions in complex **2**.

Table S5 SHAPE analysis for complex **2**.

Complex	M	PBPY-7	COC-7	CTRR-7	JPBPY
	Mn 1	**0.415**	7.055	5.235	3.147
2		PPY-6	**OC-6**	TPR-6	JPPY-6
	Mn 2	20.007	**1.282**	12.881	28.716

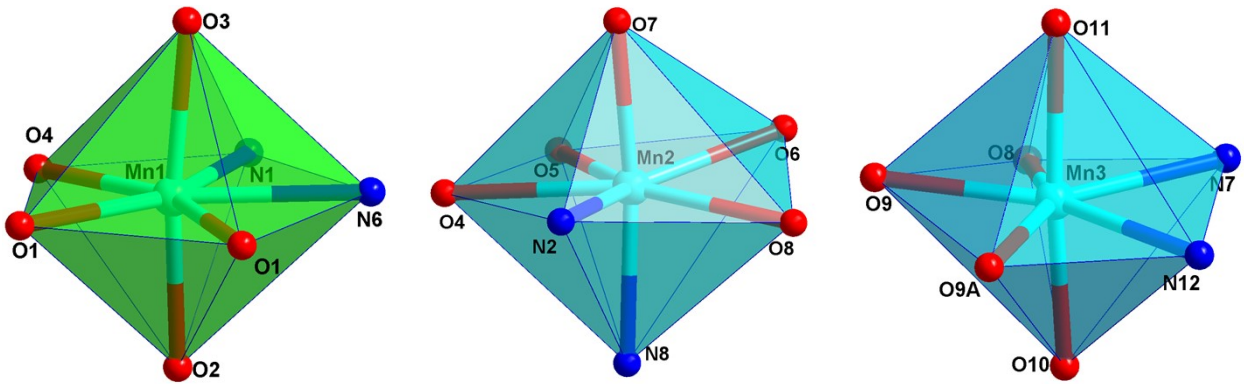

Figure S3 Local coordination geometry of Mn(II) ions in complex **3**.

Table S6 SHAPE analysis for complex **3**.

Complex	M	PBPY-7	COC-7	CTRR-7	JPBPY-7
	Mn 1	**0.261**	7.880	5.982	3.094
3	**Mn 2**	**2.652**	5.882	4.656	5.916
	Mn 3	0.989	**6.902**	5.046	3.983

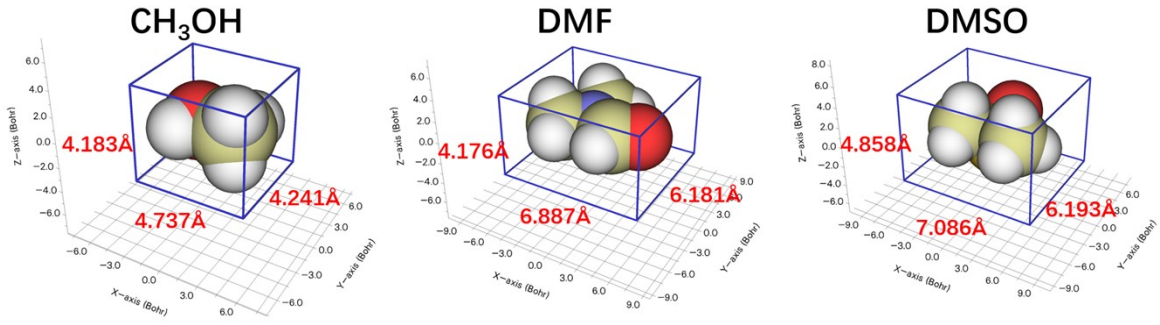

Figure S4 The size of CH_3OH, DMF and DMSO.

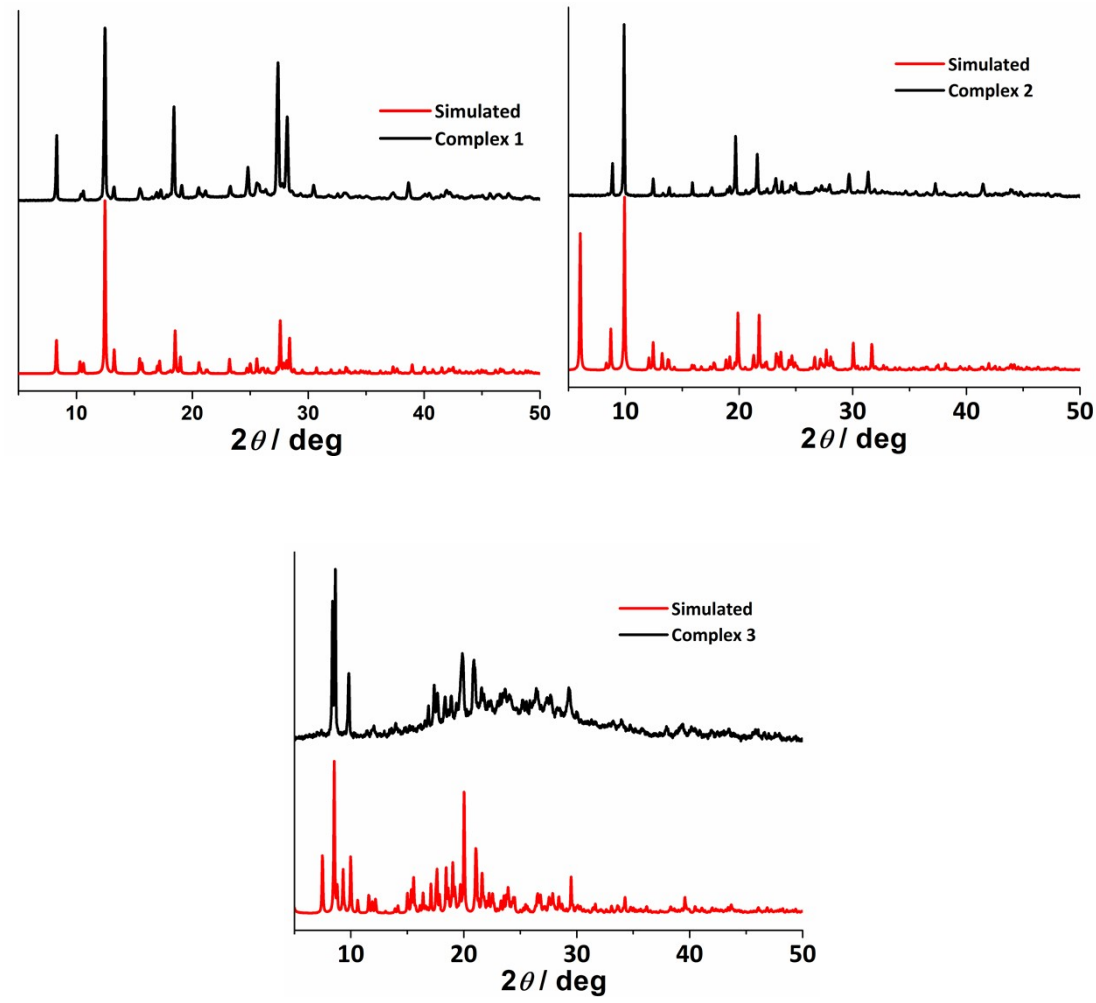

Figure S5 Powder X-ray diffraction (PXRD) patterns for complexes **1**-**3**.

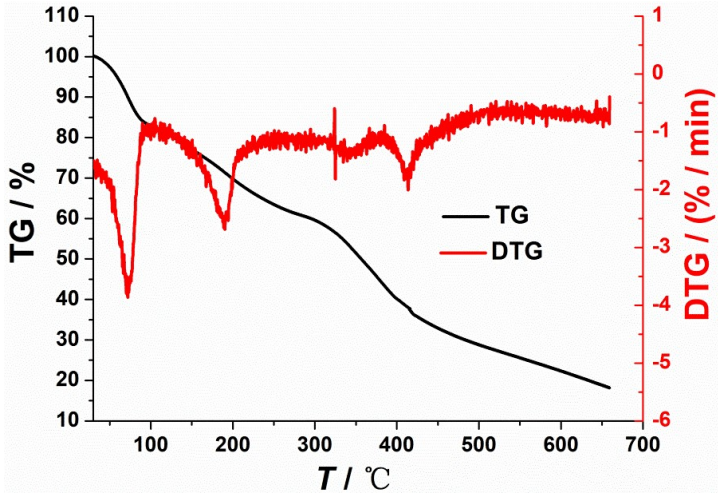

Figure S6 TG curves of complex **1** under N_2 atmosphere.

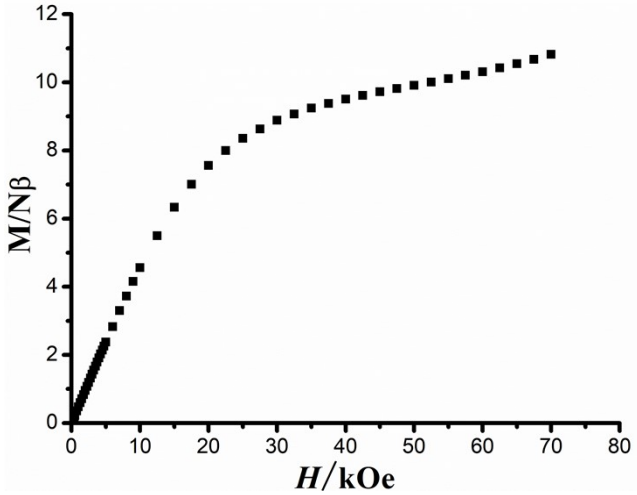

Figure S7 *M* versus *H* plot at 2 K for complex **2**.

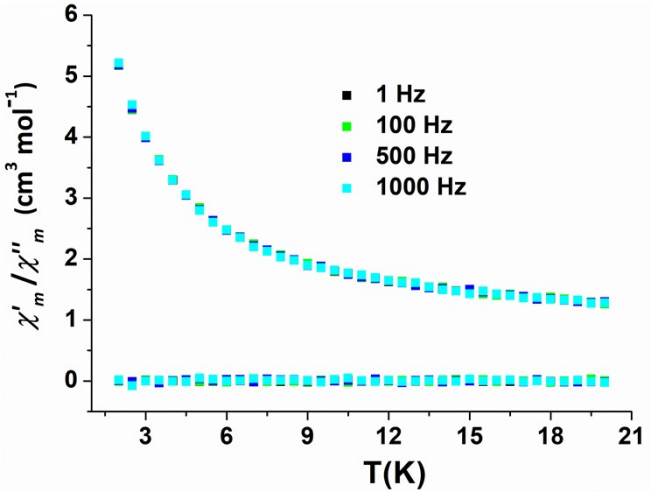

Figure S8 Temperature dependence of the in-phase and out-phase in zero field for complex **2**.

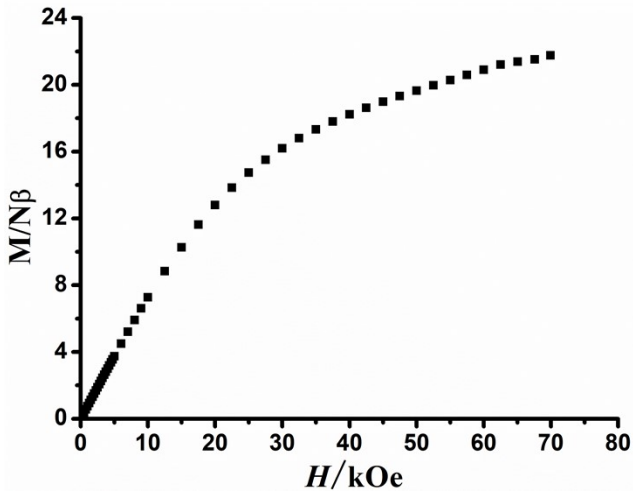

Figure S9 *M* versus *H* plot at 2 K for complex **3**.

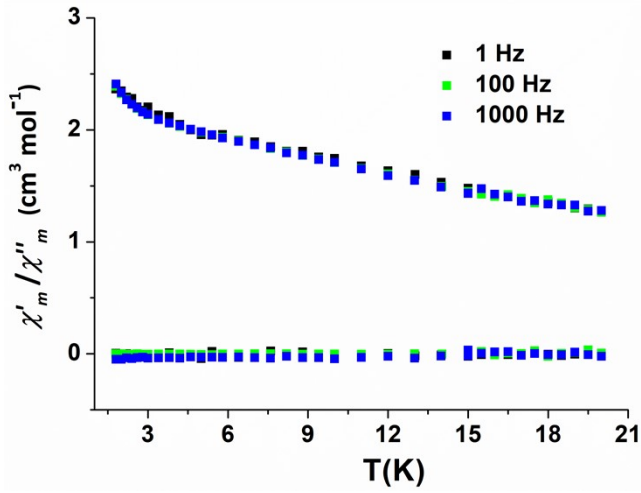

Figure S10 Temperature dependence of the in-phase and out-phase in zero field for complex **3**.

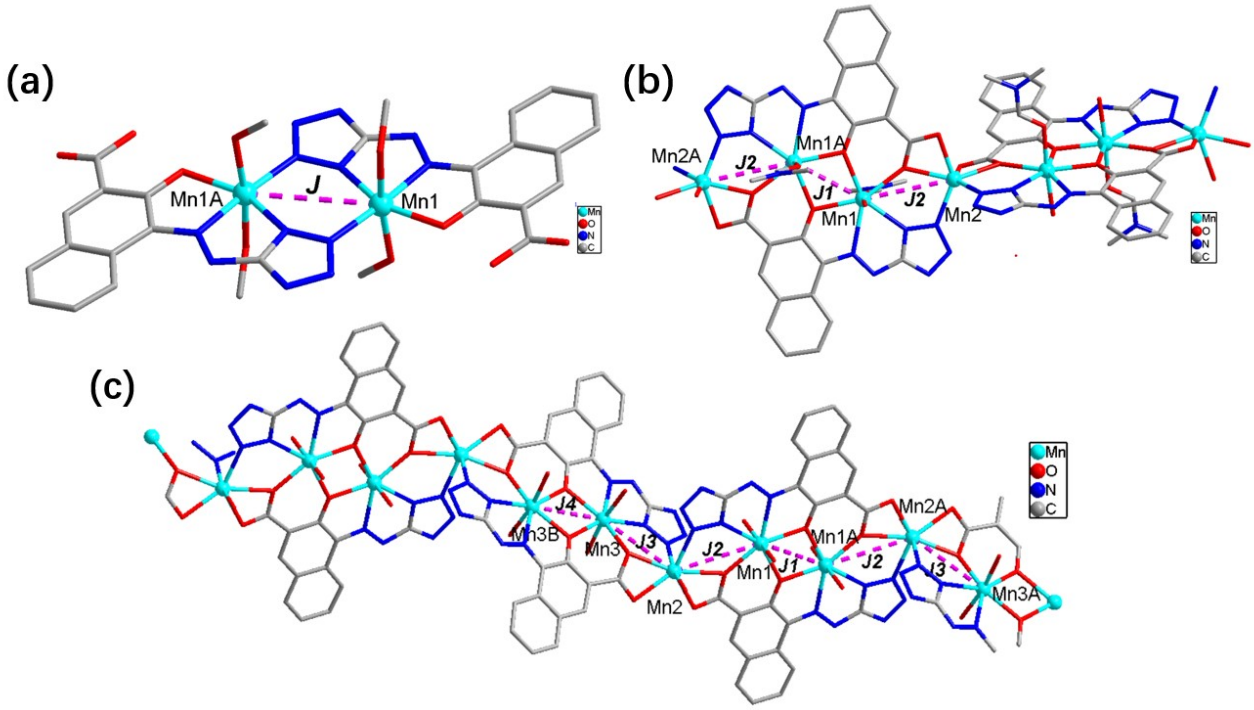

Figure S11 Magnetic exchange pathways between metal ions on the figure of X-ray structure in complexes **1**-**3**.