Electronic Supplementary Information (ESI):

Enantiomers of Conformation-Flexible Cyclopentane-1,2,3,4-tetracarboxylic acid in Metal-Organic Frameworks

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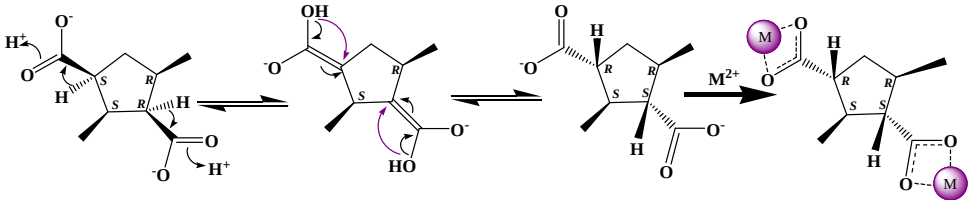


Fig. S1 Possible conformation conversion mechanism. Note: black and pink arrows represent migration of electron and proton, respectively.

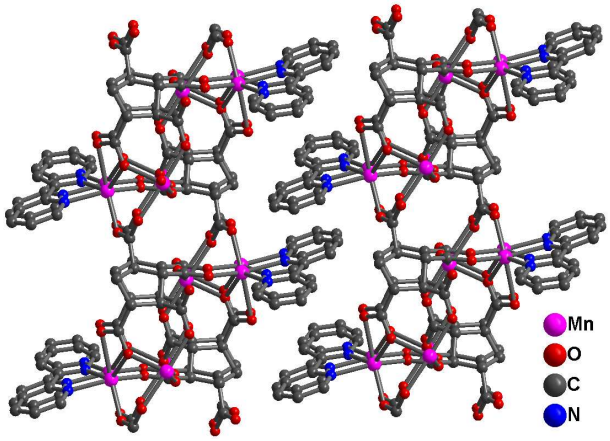


Fig. S2 View of a 2D layer structure of **1 (**2,2'-bpy ligands are projected both sides of the layer).

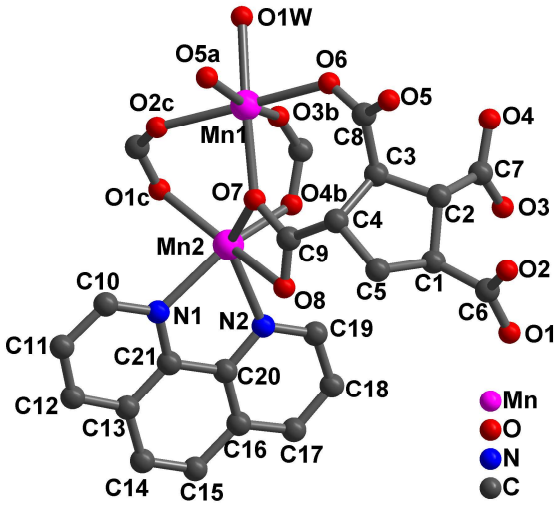


Fig. S3 View of the coordination environment of Mn atoms in **2**.

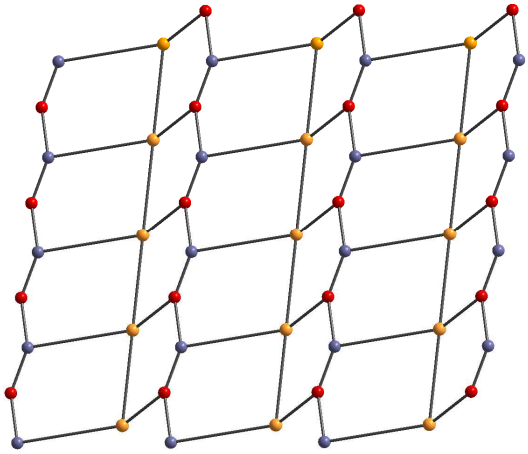


Fig. S4 View of the (3,4)-connected $(5^3)_2(5^4,8^2)$ topological layer in **3**. Note: red spheres represent Mn(1) and Mn(2) dimers, orange and purple spheres represent two different μ_5-mode cptc ligands.

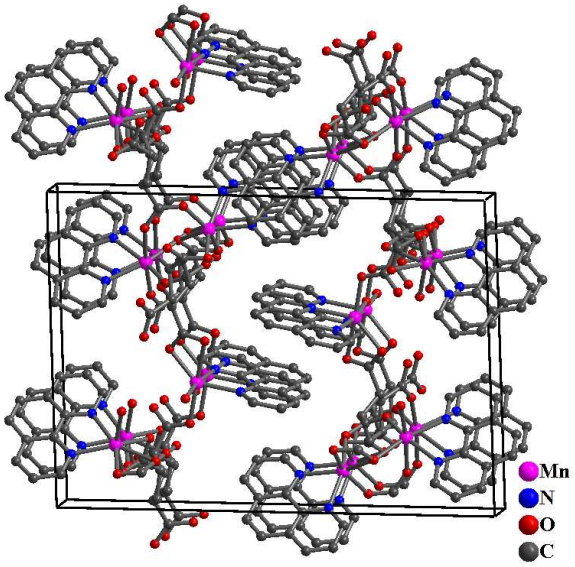


Fig. S5 View of 3D supramolecular structure of **3**.

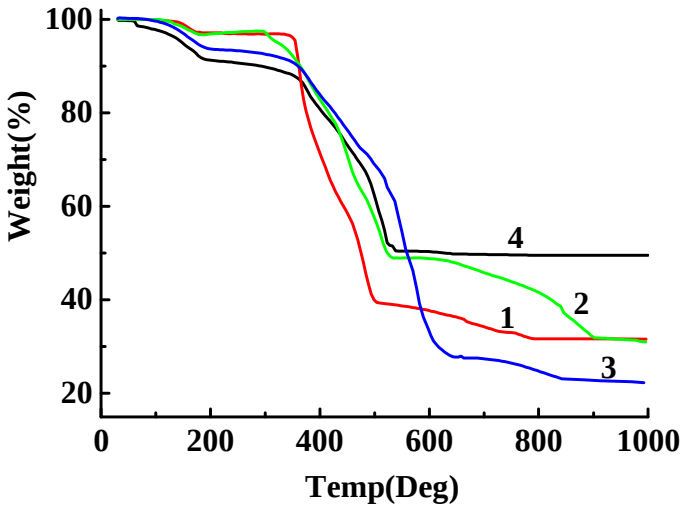
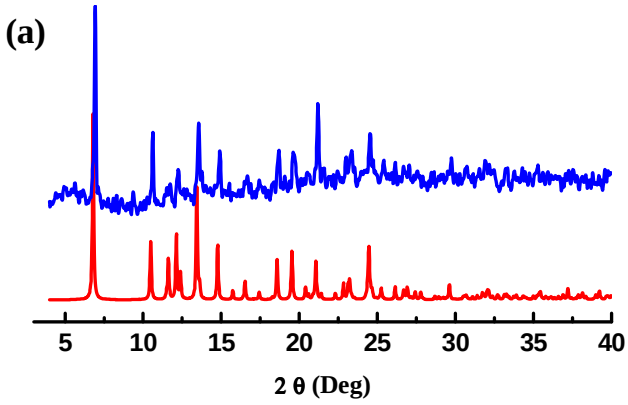


Fig. S6 TGA curves of **1-4** in air atmosphere at the heating rate of 10°C/min.



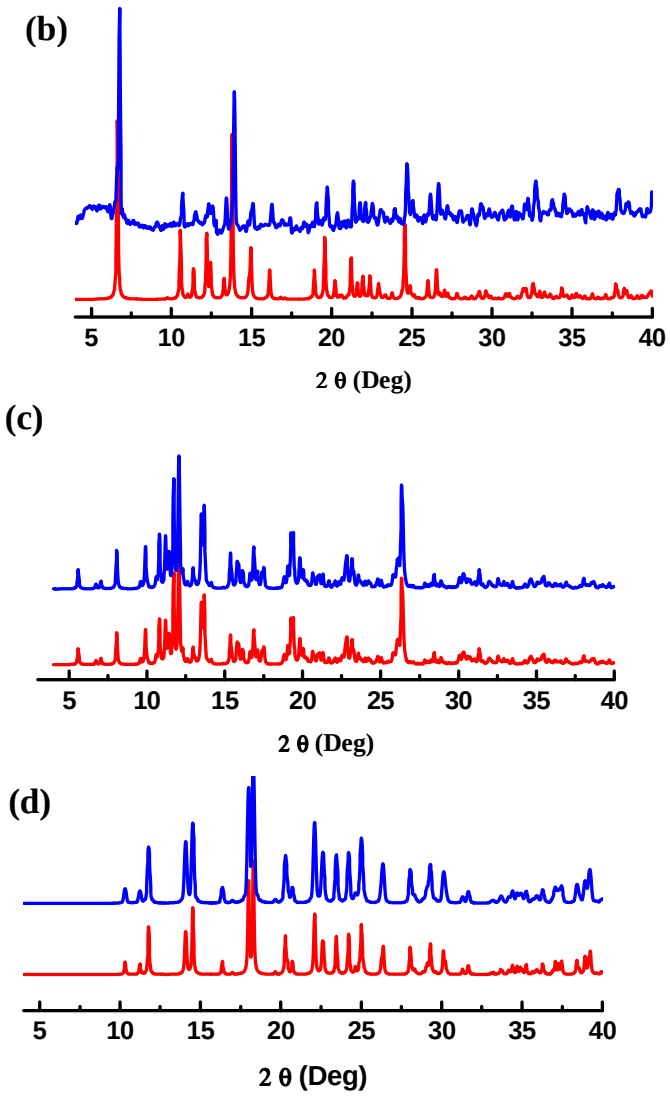


Fig. S7 Simulated (red) and experimental (blue) XPRD data for (a) **1**, (b) **2**, (c) **3** and (d) **4**.

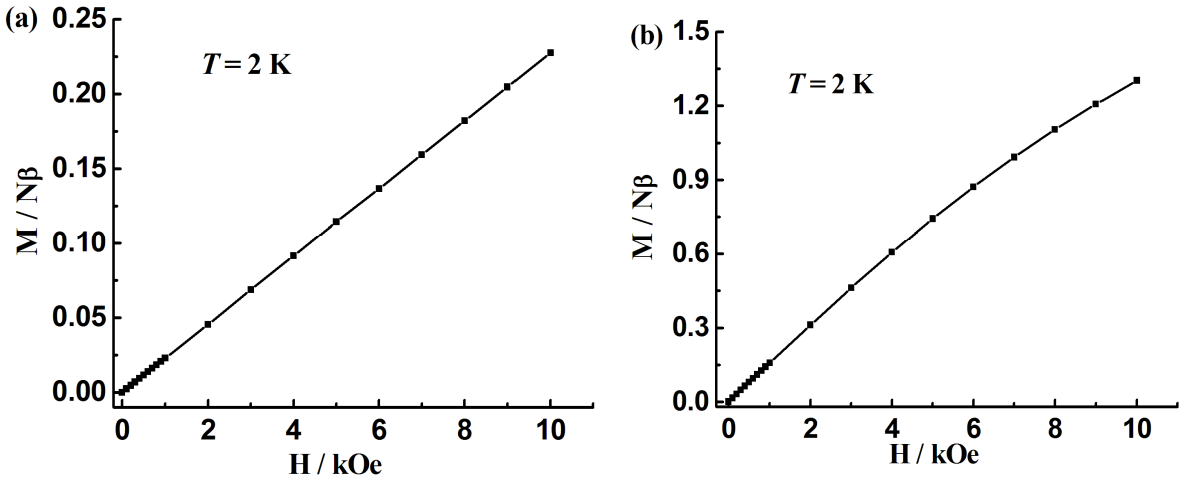


Fig S8. *M* versus *H* curve measured at 2 K (a) for **1** and (b) for **3**.

Table S1. Bond lengths [Å] and angles [deg] for **1-4**.

Compound 1

Mn(1)-O(5a)	2.1143(18)	Mn(2)-O(4)	2.1118(19)
Mn(1)-O(6b)	2.1444(19)	Mn(2)-O(1c)	2.1549(19)
Mn(1)-O(3)	2.1547(19)	Mn(2)-O(7b)	2.216(2)
Mn(1)-O(7b)	2.2060(19)	Mn(2)-N(1)	2.254(3)
Mn(1)-O(1W)	2.207(2)	Mn(2)-N(2)	2.273(3)
Mn(1)-O(2c)	2.2195(19)	Mn(2)-O(8b)	2.388(2)

O(5a)-Mn(1)-O(6b)	88.52(7)	O(4)-Mn(2)-O(1c)	92.80(8)
O(5a)-Mn(1)-O(3)	166.74(8)	O(4)-Mn(2)-O(7b)	96.08(8)
O(6b)-Mn(1)-O(3)	95.10(8)	O(1c)-Mn(2)-O(7b)	103.65(7)
O(5a)-Mn(1)-O(7b)	104.71(8)	O(4)-Mn(2)-N(1)	152.65(9)
O(6b)-Mn(1)-O(7b)	96.60(7)	O(1c)-Mn(2)-N(1)	86.64(9)
O(3)-Mn(1)-O(7b)	87.57(8)	O(7b)-Mn(2)-N(1)	110.63(9)
O(5a)-Mn(1)-O(1W)	90.35(8)	O(4)-Mn(2)-N(2)	85.58(9)
O(6b)-Mn(1)-O(1W)	88.17(8)	O(1c)-Mn(2)-N(2)	122.40(9)
O(3)-Mn(1)-O(1W)	77.05(8)	O(7b)-Mn(2)-N(2)	133.82(9)
O(7b)-Mn(1)-O(1W)	164.27(8)	N(1)-Mn(2)-N(2)	71.92(10)
O(5a)-Mn(1)-O(2c)	87.75(7)	O(4)-Mn(2)-O(8b)	98.65(9)
O(6b)-Mn(1)-O(2c)	175.54(8)	O(1c)-Mn(2)-O(8b)	157.27(9)
O(3)-Mn(1)-O(2c)	89.08(8)	O(7)-Mn(2)-O(8b)	55.80(7)
O(7b)-Mn(1)-O(2c)	82.00(7)	N(1)-Mn(2)-O(8b)	91.92(9)
O(1W)-Mn(1)-O(2c)	94.29(8)	N(2)-Mn(2)-O(8b)	78.26(9)

Symmetry codes: a) x+1,y,z; b) -x,-y+2,-z+1; c) -x,-y+1,-z+1.

Compound 2

Mn(1)-O(5a)	2.1172(14)	Mn(2)-O(4b)	2.1089(14)
Mn(1)-O(6)	2.1457(14)	Mn(2)-O(1c)	2.1623(14)
Mn(1)-O(3b)	2.1601(15)	Mn(2)-O(7)	2.1926(15)
Mn(1)-O(2c)	2.2004(14)	Mn(2)-N(1)	2.2529(18)

Mn(1)-O(7)	2.2157(14)	Mn(2)-N(2)	2.2999(19)
Mn(1)-O(1W)	2.2179(16)	Mn(2)-O(8)	2.4604(19)

O(5a)-Mn(1)-O(6)	87.90(6)	O(4b)-Mn(2)-O(1c)	92.41(6)
O(5a)-Mn(1)-O(3b)	167.95(6)	O(4b)-Mn(2)-O(7)	94.81(6)
O(6)-Mn(1)-O(3b)	95.26(6)	O(1c)-Mn(2)-O(7)	101.50(5)
O(5a)-Mn(1)-O(2c)	86.22(5)	O(4b)-Mn(2)-N(1)	146.43(7)
O(6)-Mn(1)-O(2c)	173.84(6)	O(1c)-Mn(2)-N(1)	84.84(6)
O(3b)-Mn(1)-O(2c)	90.88(6)	O(7)-Mn(2)-N(1)	118.56(7)
O(5a)-Mn(1)-O(7)	104.74(6)	O(4b)-Mn(2)-N(2)	82.31(6)
O(6)-Mn(1)-O(7)	96.73(5)	O(1c)-Mn(2)-N(2)	126.08(6)
O(3b)-Mn(1)-O(7)	86.47(6)	O(7)-Mn(2)-N(2)	132.37(6)
O(2c)-Mn(1)-O(7)	83.01(5)	N(1)-Mn(2)-N(2)	72.73(7)
O(5a)-Mn(1)-O(1W)	92.21(6)	O(4b)-Mn(2)-O(8)	105.04(7)
O(6)-Mn(1)-O(1W)	88.39(6)	O(1c)-Mn(2)-O(8)	151.06(7)
O(3b)-Mn(1)-O(1W)	76.30(6)	O(7)-Mn(2)-O(8)	54.90(5)
O(2c)-Mn(1)-O(1W)	93.67(6)	N(1)-Mn(2)-O(8)	92.46(7)
O(7)-Mn(1)-O(1W)	162.42(6)	N(2)-Mn(2)-O(8)	79.82(7)

Symmetry codes: a) -x+3,-y+2,-z+1; b)-x+4,-y+2,-z+1; c) x,y+1,z .

Compound 3

Mn(1)-O(6a)	2.118(5)	Mn(3)-O(2W)	2.122(6)
Mn(1)-O(2)	2.121(5)	Mn(3)-O(16)	2.226(5)
Mn(1)-O(8a)	2.186(4)	Mn(3)-O(12b)	2.268(7)
Mn(1)-O(9)	2.211(5)	Mn(3)-N(6)	2.277(6)
Mn(1)-N(1)	2.269(5)	Mn(3)-O(15)	2.315(5)
Mn(1)-N(2)	2.295(5)	Mn(3)-N(5)	2.316(6)
Mn(2)-O(10)	2.082(4)	Mn(3)-O(11b)	2.421(7)
Mn(2)-O(1)	2.110(4)	Mn(4)-O(3)	2.157(5)
Mn(2)-O(8a)	2.186(5)	Mn(4)-O(1W)	2.161(6)
Mn(2)-N(4)	2.222(5)	Mn(4)-O(13c)	2.162(7)

Mn(2)-N(3)	2.280(5)	Mn(4)-N(7)	2.238(7)
Mn(2)-O(7a)	2.474(5)	Mn(4)-N(8)	2.269(7)
		Mn(4)-O(4)	2.456(6)

O(6a)-Mn(1)-O(2)	93.76(19)	O(2W)-Mn(3)-N(6)	103.8(2)
O(6a)-Mn(1)-O(8a)	90.47(17)	O(16)-Mn(3)-N(6)	95.9(2)
O(2)-Mn(1)-O(8a)	103.58(18)	O(12b)-Mn(3)-N(6)	80.8(2)
O(6a)-Mn(1)-O(9)	174.10(18)	O(2W)-Mn(3)-O(15)	100.8(2)
O(2)-Mn(1)-O(9)	85.25(19)	O(16)-Mn(3)-O(15)	57.05(18)
O(8a)-Mn(1)-O(9)	84.12(17)	O(12b)-Mn(3)-O(15)	124.8(2)
O(6a)-Mn(1)-N(1)	87.64(18)	N(6)-Mn(3)-O(15)	143.8(2)
O(2)-Mn(1)-N(1)	92.15(19)	O(2W)-Mn(3)-N(5)	82.1(2)
O(8a)-Mn(1)-N(1)	164.25(18)	O(16)-Mn(3)-N(5)	94.9(2)
O(9)-Mn(1)-N(1)	98.21(17)	O(12b)-Mn(3)-N(5)	149.1(2)
O(6a)-Mn(1)-N(2)	100.50(19)	N(6)-Mn(3)-N(5)	71.6(2)
O(2)-Mn(1)-N(2)	158.63(18)	O(15)-Mn(3)-N(5)	86.1(2)
O(8a)-Mn(1)-N(2)	92.21(18)	O(2W)-Mn(3)-O(11b)	82.3(2)
O(9)-Mn(1)-N(2)	82.11(18)	O(16)-Mn(3)-O(11b)	91.6(2)
N(1)-Mn(1)-N(2)	72.80(18)	O(12b)-Mn(3)-O(11b)	52.4(2)
O(10)-Mn(2)-O(1)	96.15(18)	N(6)-Mn(3)-O(11b)	133.1(2)
O(10)-Mn(2)-O(8a)	95.02(17)	O(15)-Mn(3)-O(11b)	76.1(2)
O(1)-Mn(2)-O(8a)	97.41(18)	N(5)-Mn(3)-O(11b)	153.6(2)
O(10)-Mn(2)-N(4)	116.23(19)	O(3)-Mn(4)-O(1W)	98.5(3)
O(1)-Mn(2)-N(4)	91.83(19)	O(3)-Mn(4)-O(13c)	129.4(3)
O(8a)-Mn(2)-N(4)	146.26(18)	O(1W) -Mn(4)-O(13c)	83.1(3)
O(10)-Mn(2)-N(3)	89.59(19)	O(3)-Mn(4)-N(7)	140.3(2)
O(1)-Mn(2)-N(3)	165.01(19)	O(1W)-Mn(4)-N(7)	96.9(3)
O(8a)-Mn(2)-N(3)	95.87(18)	O(13c)-Mn(4)-N(7)	88.7(3)
N(4)-Mn(2)-N(3)	73.2(2)	O(3)-Mn(4)-N(8)	90.5(2)
O(10)-Mn(2)-O(7a)	148.15(18)	O(1W)-Mn(4)-N(8)	170.1(3)

O(1)-Mn(2)-O(7a)	99.43(17)	O(13c)-Mn(4)-N(8)	94.5(3)
O(8a)-Mn(2)-O(7a)	55.60(15)	N(7)-Mn(4)-N(8)	73.5(3)
N(4)-Mn(2)-O(7a)	90.93(18)	O(3)-Mn(4)-O(4)	56.63(19)
N(3)-Mn(2)-O(7a)	82.41(18)	O(1W)-Mn(4)-O(4)	83.8(2)
O(2W)-Mn(3)-O(16)	157.9(2)	O(13c)-Mn(4)-O(4)	166.4(2)
O(2W)-Mn(3)-O(12b)	91.4(3)	N(7)-Mn(4)-O(4)	89.1(2)
O(16)-Mn(3)-O(12b)	101.7(2)	N(8)-Mn(4)-O(4)	97.8(2)

Symmetry codes: a) x+1,y,z; b) x-1,y,z; c) x,y-1,z.

Compound 4

Cd(1)-O(8)	2.233(4)	Cd(2)-O(2W)	2.245(4)
Cd(1)-O(5a)	2.300(4)	Cd(2)-O(7)	2.255(4)
Cd(1)-O(4b)	2.358(4)	Cd(2)-O(3W)	2.260(5)
Cd(1)-O(2c)	2.394(4)	Cd(2)-O(1d)	2.300(4)
Cd(1)-O(3b)	2.409(4)	Cd(2)-O(6)	2.306(5)
Cd(1)-O(1c)	2.481(4)	Cd(2)-O(1W)	2.327(5)

O(8)-Cd(1)-O(5a)	101.45(17)	O(2W)-Cd(2)-O(7)	88.22(17)
O(8)-Cd(1)-O(4b)	145.44(15)	O(2W)-Cd(2)-O(3W)	82.87(19)
O(5a)-Cd(1)-O(4b)	92.27(15)	O(7)-Cd(2)-O(3W)	87.26(16)
O(8)-Cd(1)-O(2c)	86.81(16)	O(2W)-Cd(2)-O(1d)	92.93(16)
O(5a)-Cd(1)-O(2c)	142.37(15)	O(7)-Cd(2)-O(1d)	173.83(16)
O(4b)-Cd(1)-O(2c)	101.45(16)	O(3W)-Cd(2)-O(1d)	86.87(16)
O(8)-Cd(1)-O(3b)	94.93(15)	O(2W)-Cd(2)-O(6)	84.55(18)
O(5a)-Cd(1)-O(3b)	134.71(15)	O(7)-Cd(2)-O(6)	88.53(16)
O(4b)-Cd(1)-O(3b)	54.68(14)	O(3W)-Cd(2)-O(6)	166.85(17)
O(2c)-Cd(1)-O(3b)	79.84(15)	O(1d)-Cd(2)-O(6)	97.61(16)
O(8)-Cd(1)-O(1c)	120.14(15)	O(2W)-Cd(2)-O(1W)	167.5(2)
O(5a)-Cd(1)-O(1c)	92.39(15)	O(7)-Cd(2)-O(1W)	94.25(18)
O(4b)-Cd(1)-O(1c)	90.40(15)	O(3W)-Cd(2)-O(1W)	85.05(19)
O(2c)-Cd(1)-O(1c)	53.13(14)	O(1d)-Cd(2)-O(1W)	83.36(16)

O(3b)-Cd(1)-O(1c)	115.10(15)	O(6)-Cd(2)-O(1W)	107.70(18)

Symmetry codes: a)-x+1,y-1/2,-z+1/2; b) x,y-1,z; c) -x,-y+2,-z; d) x,-y+5/2,z+1/2.

Table S2. Free energies of the conformations and △G values compared with conformation I.

	gas phase		solvate in water	
	a.u	kcal mol $^{-1}$(△G)	a.u	kcal mol $^{-1}$(△G)
I	-947.783003	0	-948.81537	0
II	-947.802100	-11.98356	-948.82972	-9.00294
III	-947.807459	-15.34638	-948.83171	-10.25577
IV	-947.808931	-16.27008	-948.83264	-10.83946
V	-947.808913	-16.25878	-948.8331	-11.12817
VI	-947.817890	-21.89194	-948.83802	-14.21133
VII	-947.817880	-21.88567	-948.83826	-14.36505
VIII	-947.818226	-22.10278	-948.8395	-15.14217
IX	-947.825905	-26.92143	-948.84606	-19.26082
X	-947.825904	-26.92081	-948.84606	-19.26019