Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information for

A water stable molecular cadmium phosphonate bearing 2-(2-pyridyl)benzimidazole as a highly sensitive luminescence sensor for selective detection of bisphenol AF and bisphenol B

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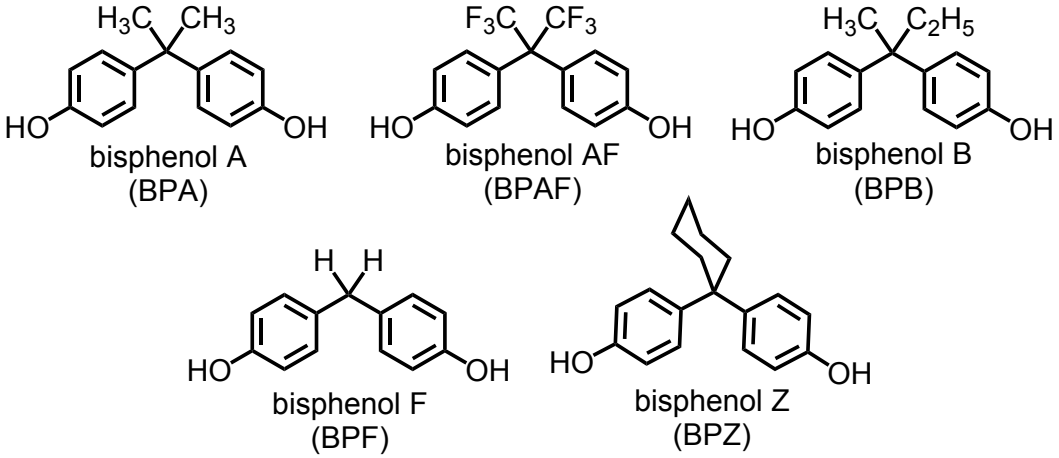
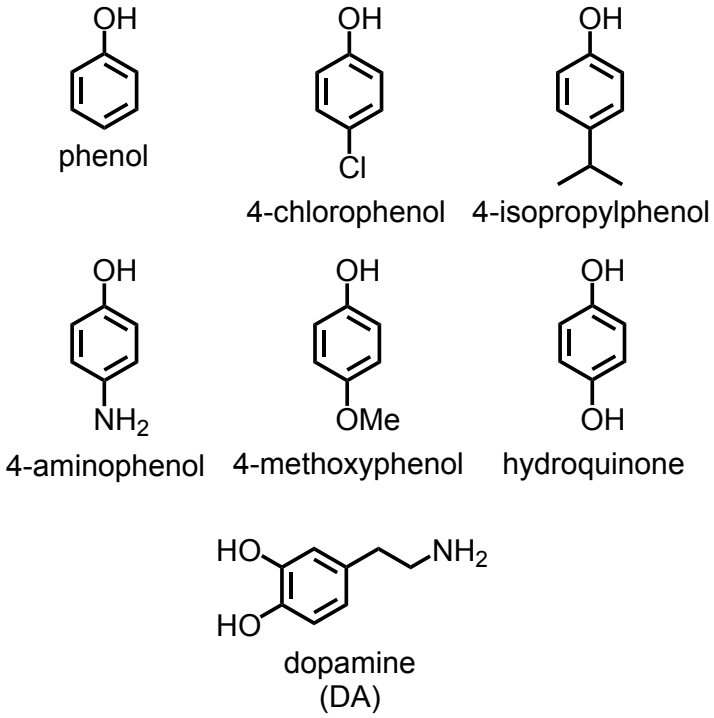


Scheme S1. Molecular structures of bisphenol analogues



Scheme S2. Molecular structures of phenol derivatives and dopamine

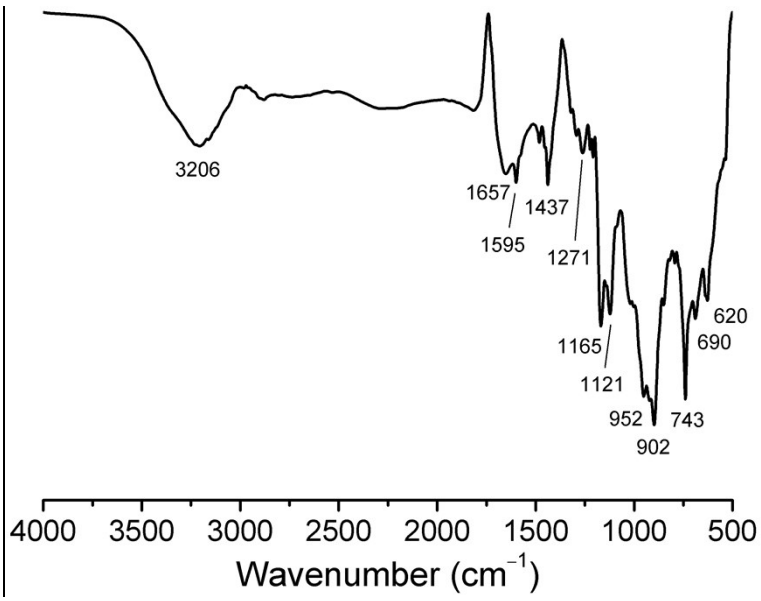


Fig. S1 IR spectra of **1**·2H_2O.

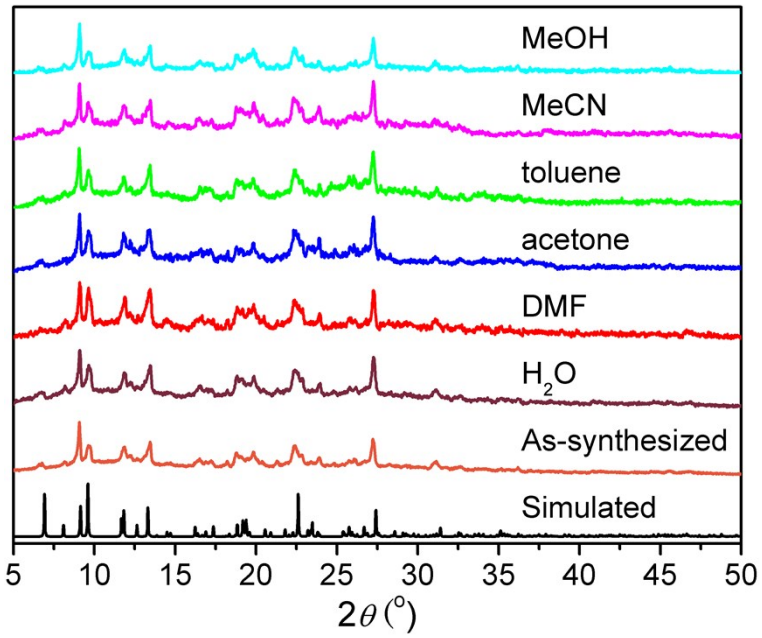


Fig. S2 Simulated and experimental PXRD patterns of **1**·2H_2O before and after immersing in H_2O, DMF, acetone, toluene, MeCN, and MeOH for 24 h.

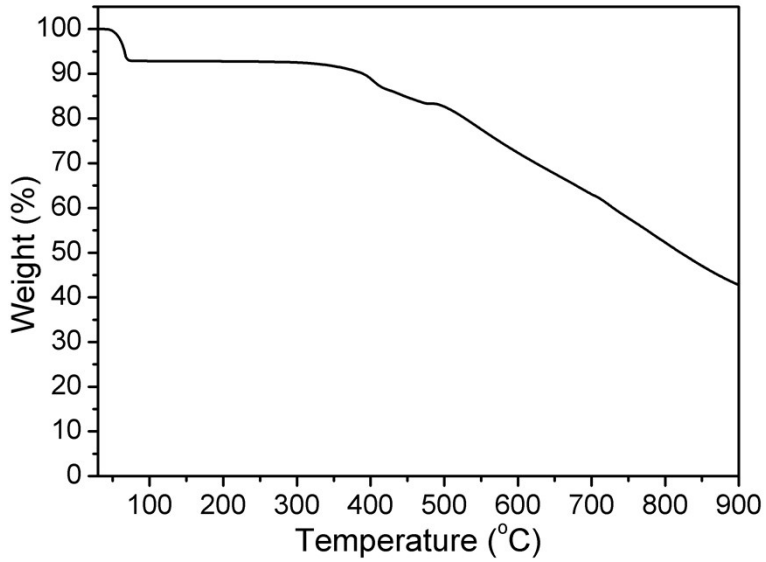


Fig. S3 TG diagram of **1**·2H_2O.

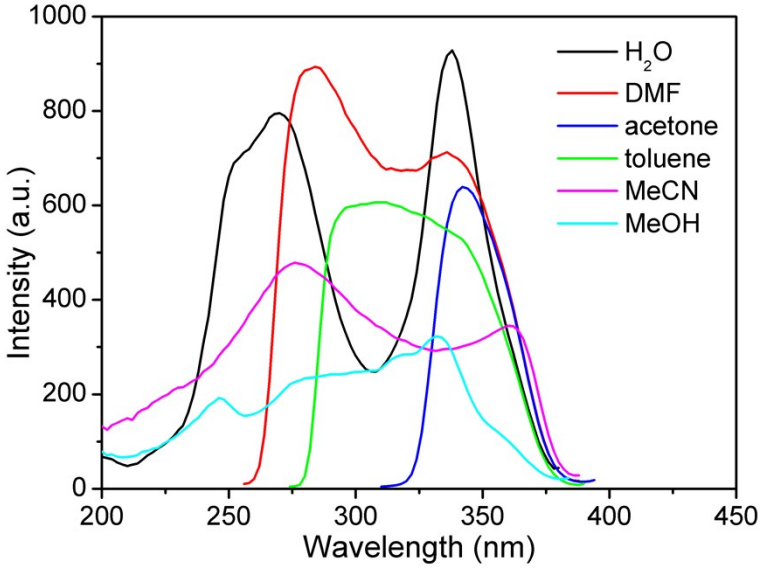


Fig. S4 Excitation spectra of **1**·2H_2O in different solvent suspensions at room temperature.

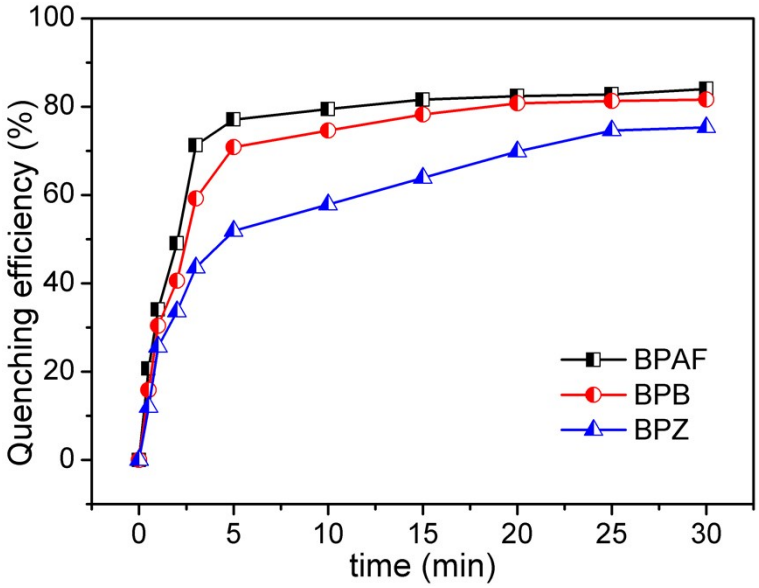


Fig. S5 The response time of **1**·2H_2O in H_2O suspensions to monitor the bisphenols, including BPAF, BPB, and BPZ.

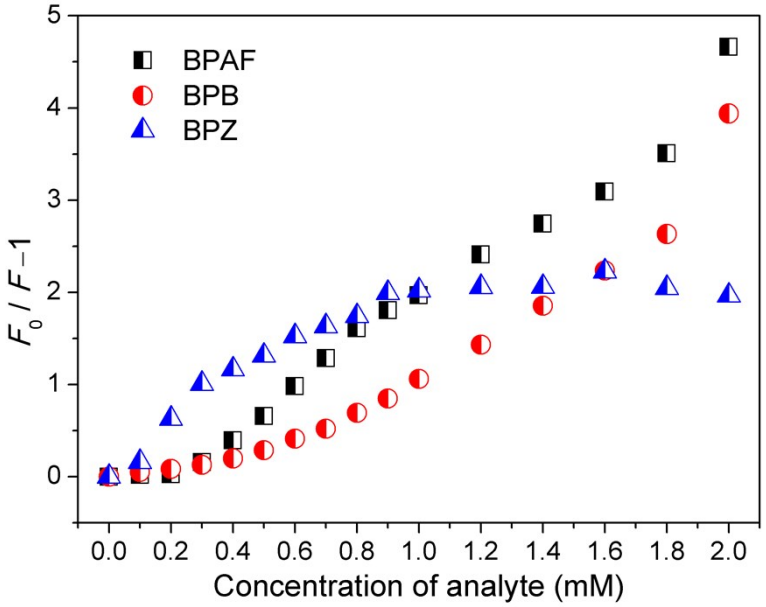
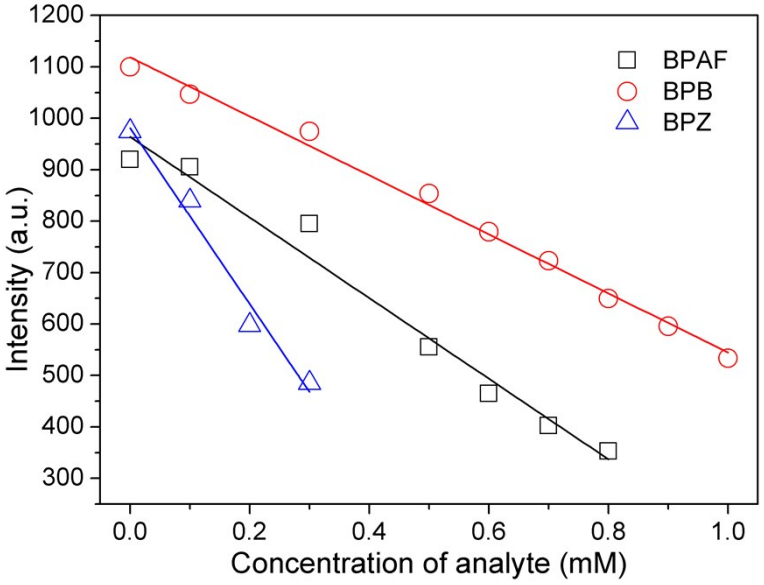


Fig. S6 Stern–Volmer plots for the luminescence detection of **1**·2H_2O toward BPAF, BPB, and BPZ in the full titration concentrations.



	BPAF	BPB	BPZ
Blank reading 1	913.7	1104	972.2
Blank reading 2	915.4	1098	975.8
Blank reading 3	920.6	1097	976.5
Blank reading 4	920.7	1098	976.0
Blank reading 5	920.3	1100	974.6
Standard deviation (σ)	***3.335***	***2.793***	***1.724***
$\lvert$ ***Slope*** $\rvert$ ***(k), mM^{-1}***	783.79	573.96	1709.3
R^2	0.97164	0.99243	0.97074
LOD ($3\sigma/k$), μM	**12.8**	**14.6**	**3.0**

Fig. S7 Linear plots of luminescence intensity against concentration of analyte (BPAF, BPB, and BPZ) for **1**·2H_2O in H_2O suspensions in the low concentration region at room temperature when excited at λ_{ex} = 340 nm.

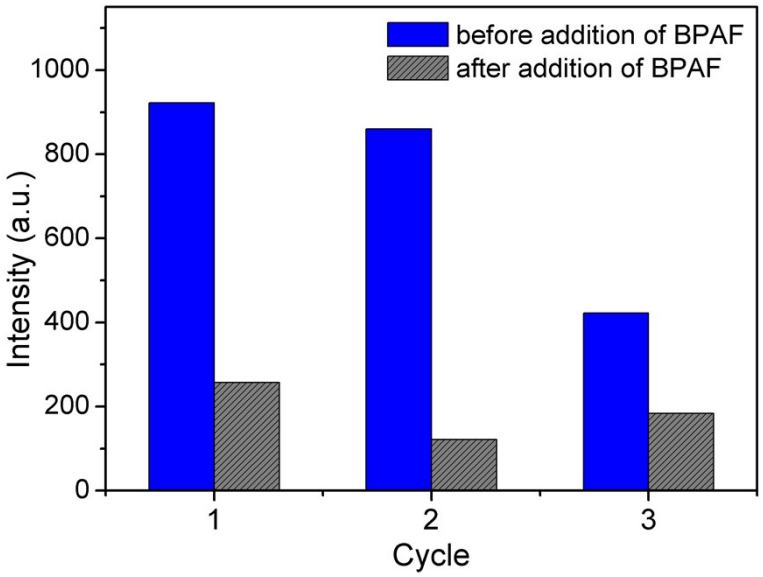


Fig. S8 Reusability of **1**·2H_2O for luminescence detection of BPAF in H_2O for 3 cycles.

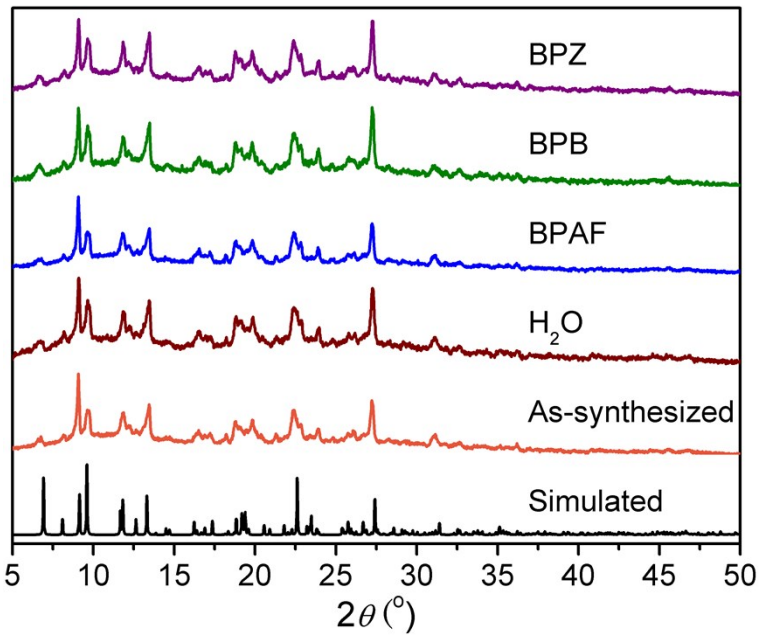


Fig. S9 PXRD patterns of **1**·2H_2O before and after treated with BPAF, BPB, and BPZ in water for 24 h.

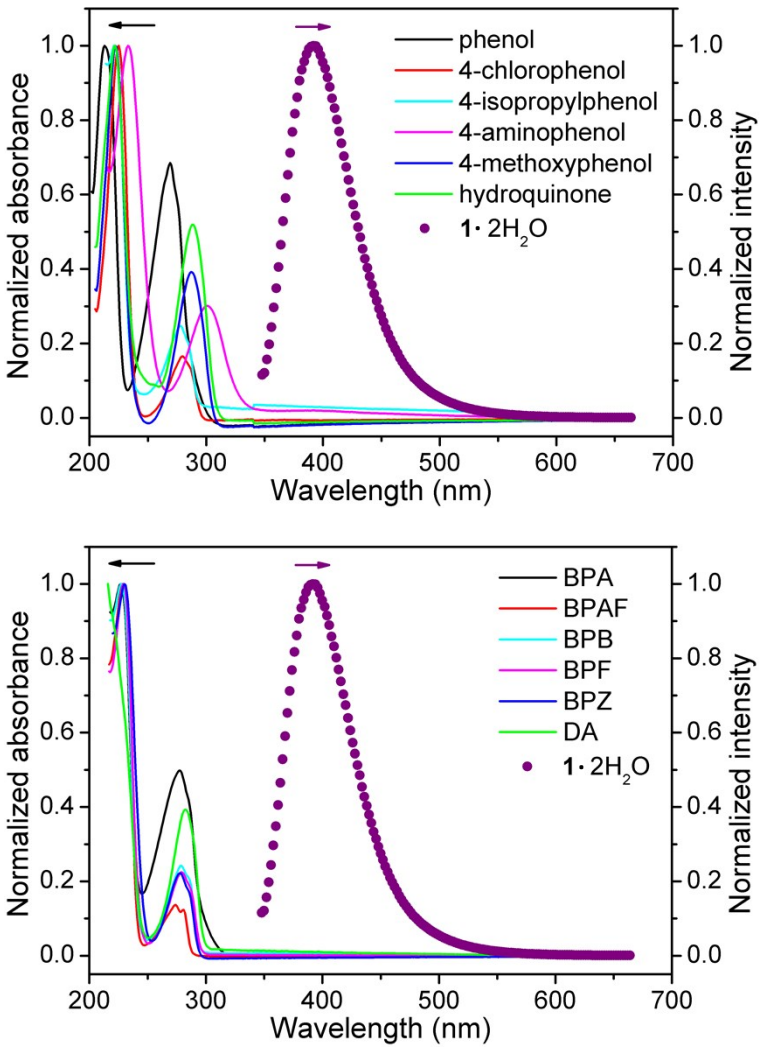
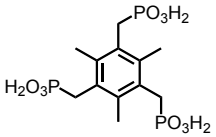
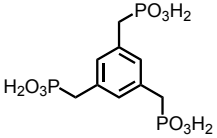
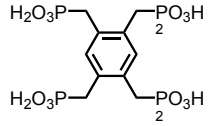
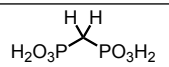
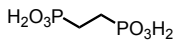
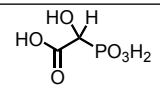
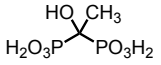
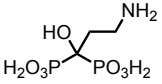


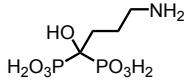
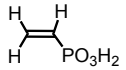
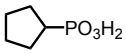
Fig. S10 Normalized absorption spectra of phenolic analytes in aqueous solutions (solid lines) and normalized emission spectrum of $\mathbf{1}\cdot 2H_2O$ in H_2O suspension (dotted curve), showing no spectral overlap.

Table S1. Hydrogen-bonding parameter (Å, °) for **1**·2H_2O□

D−H···A	*d*(D−H)	*d*(H···A)	*d*(D···A)	<D−H···A	Symmetry code
Between the Hpybim ligands and the lattice water molecules					
N2−H2A···O12	0.88	2.06	2.944(7)	180	
Between the phosphonate groups themselves					
O3−H101···O2	0.84	1.73	2.564(5)	173	$1-x, 1-y, 1-z$
O6−H102···O3	0.84	2.02	2.790(6)	152	$1-x, 1-y, 1-z$
O8−H103···O4	0.84	1.72	2.522(6)	160	$x, 1+y, z$
O9−H104···O2	0.84	1.70	2.506(6)	159	$1-x, 1-y, 1-z$
Between the aqua ligands and the phosphonate groups					
O10−H105···O5	0.83	1.85	2.663(6)	167	$1-x, 1-y, 1-z$
O10−H106···O5	0.83	1.95	2.730(6)	158	$-1+x, y, -1+z$
O11−H107···O4	0.83	1.96	2.778(6)	170	$-1+x, y, -1+z$
Between the lattice water molecules and the phosphonate groups					
O12−H109···O7	0.83	2.00	2.825(6)	175	$2-x, 1-y, 1-z$
O12−H110···O4	0.82	2.07	2.888(6)	171	$x, y, -1+z$
Between the aqua ligands and the lattice water molecules					
O11−H108···O12	0.83	1.91	2.730(6)	176	$1-x, -y, -z$

Table S2. Comparison on three-component metal phosphonates incorporating secondary auxiliary N,N-heterocyclic chelators

Compound	Phosphonate	N,N-chelator	Structure properties	ref
$[Cd_2(H_4tpmm)_2(Hpybim)_2(H_2O)_4]\cdot 2H_2O$ (**1**·2H$_2$O)		Hpybim	0D M_2L_2	This work
$[Cu_2(H_4tpmm)_2(2,2'\text{-bipy})_2(H_2O)_2]\cdot H_2O$		2,2′-bipy	0D M_2L_2	S1
$[Ni_2(H_4tpmm)_2(2,2'\text{-bipy})_2(H_2O)_4]$		2,2′-bipy	0D M_2L_2	S1
$[Co_2(H_4tpmm)_2(2,2'\text{-bipy})_2(H_2O)_4]$		2,2′-bipy	0D M_2L_2	S1
$[Cu_2(H_4bmt)_2(2,2'\text{-bipy})_2(H_2O)_4]$		2,2′-bipy	0D M_2L_2	S2
$[Cd_2(H_4bmt)_2(2,2'\text{-bipy})_2]\cdot 4H_2O$		2,2′-bipy	0D M_2L_2	S3
$[Zn(H_4bmt)(2,2'\text{-bipy})]_n$		2,2′-bipy	1D chain	S3
$[Co_2(H_6tpmb)_2(2,2'\text{-bipy})_2(H_2O)_2]$		2,2′-bipy	0D M_2L_2	S4
$[Zn_2(H_6tpmb)_2(2,2'\text{-bipy})_2]$		2,2′-bipy	0D M_2L_2	S4
$[Co_2(H_4tpmb)(phen)_2(H_2O)_6]\cdot 2H_2O$		phen	0D M_2L	S5
$[Ni_2(H_4tpmb)(phen)_2(H_2O)_6]\cdot 2H_2O$		phen	0D M_2L	S5
$[Co_2(H_6tpmb)_2(phen)_2(H_2O)_2]$		phen	0D M_2L_2	S5
$\{[Cu(H_2MDPA)(phen)]\cdot H_2O]\}_n$		phen	1D chain	S6
$[Cu_2(H_2EDPA)_2(phen)_2(H_2O)_4]_n$		phen	1D chain	S6
$[Co_2(H_2EDPA)_2(phen)_2(H_2O)_4]_n$		phen	1D chain	S6
$[Mn(H_2EDPA)(2,2'\text{-bipy})(H_2O)_2]_n$		2,2′-bipy	1D chain	S6
$[Zn(H_2EDPA)(2,2'\text{-bipy})]_n$		2,2′-bipy	2D layer	S6
$[Cu_2(H_2EDPA)_2(2,2'\text{-bipy})_2(H_2O)_2]\cdot 3H_2O$		2,2′-bipy	0D M_2L_2	S7
$[Cu_2(EDPA)(phen)_2(H_2O)_2]\cdot 9H_2O$		phen	0D M_2L	S8
$[Cu(HPAA)(2,2'\text{-bipy})(H_2O)]\cdot H_2O$		2,2′-bipy	mononuclear ML	S7
$[Cu(H_2EDP)(2,2'\text{-bipy})(H_2O)]\cdot 2H_2O$		2,2′-bipy	mononuclear ML	S7
$[CuCl(H_3ALE)(2,2'\text{-bipy})]\cdot 4H_2O$		2,2′-bipy	mononuclear ML	S7

$[CuCl(H_3PAM)(2,2'\text{-bipy})(H_2O)]\cdot H_2O$		2,2′-bipy	mononuclear ML	S7
$[Cu_2(VPA)_2(phen)_2(H_2O)_2]\cdot 8H_2O$		phen	0D M_2L_2	S9
$[Cu_6(C_5H_9PO_3)_4(2,2'\text{-bipy})_6(MeOH)_4](ClO_4)_4$		2,2′-bipy	0D M_6L_4	S10
$[Cu_3(C_5H_9PO_3)_2(2,2'\text{-bipy})_3(MeOH)(H_2O)](ClO_4)_2$		2,2′-bipy	0D M_3L_2	S11

Abbreviation: Hpybim = 2-(2-pyridyl)benzimidazole; 2,2′-bipy = 2,2′-bipyridine; phen = 1,10-phenanthroline; H_6tpmm = 2,4,6-tris(phosphorylmethyl)mesitylene; H_6bmt = benzene-1,3,5-triyltris(methylene))triphosphonic acid; H_8tpmb = 1,2,4,5-tetrakis(phosphorylmethyl)benzene; H_4MDPA = methanediphosphonic acid; H_4EDPA = 1,2-ethanediphosphonic acid; H_3PAA = hydroxyphosphonoacetic acid; H_4EDP = hydroxyethylidene-diphosphonic acid; H_4PAM = pamidronic acid; H_4ALE = alendronic acid; H_2VPA = vinylphosphonic acid; $C_5H_9PO_3H_2$ = cyclopentyl phosphonic acid.

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