Supporting Information

Fluorescent Selectivity for Small Molecules of Three Zn-MOFs with different Topologies Based on a Tetracarboxylate Ligand

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1. Selected Bond Lengths and Angles

Table S1: The selected bond distances (Å) and angles (deg) for complex **1**[a].

Zn1—O4	2.055 (4)	Zn2—O7^{i}	2.016 (4)
Zn1—O2	2.082 (5)	Zn2—O9	2.061 (4)
Zn1—O9^{iii}	2.134 (4)	Zn2—O6^{i}	1.975 (4)
Zn1—O1	2.170 (5)	Zn2—O11	2.046 (4)
Zn1—O3	2.101 (5)	Zn2—O8^{ii}	2.306 (5)
Zn1—O5	2.101 (4)	Zn2—O10	2.422 (4)
O9—Zn1^{i}	2.134 (4)	O6—Zn2^{iii}	1.975 (4)
O7—Zn2^{iii}	2.016 (4)	O8—Zn2^{iv}	2.306 (5)
O4—Zn1—O2	84.0 (2)	O7^{i}—Zn2—O9	104.00 (17)
O4—Zn1—O9^{iii}	91.70 (16)	O7^{i}—Zn2—O11	99.24 (18)
O4—Zn1—O1	89.23 (19)	O7^{i}—Zn2—O8^{ii}	89.68 (18)
O4—Zn1—O3	171.7 (2)	O7^{i}—Zn2—O10	159.97 (18)
O4—Zn1—O5	96.5 (2)	O7^{i}—Zn2—C21	132.1 (2)

O2—Zn1—O9^{iii}	92.28 (19)	O7^{i}—Zn2—C1^{ii}	95.5 (2)
O2—Zn1—O1	93.6 (2)	O9—Zn2—O8^{ii}	88.92 (15)
O2—Zn1—O3	89.6 (2)	O9—Zn2—O10	57.99 (16)
O2—Zn1—O5	177.9 (2)	O9—Zn2—C21	29.34 (17)
O9^{iii}—Zn1—O1	174.14 (18)	O9—Zn2—C1^{ii}	116.0 (2)
O3—Zn1—O9^{iii}	93.81 (17)	O6^{i}—Zn2—O7^{i}	99.23 (19)
O3—Zn1—O1	85.9 (2)	O6^{i}—Zn2—O9	106.98 (17)
O3—Zn1—O5	89.65 (19)	O6^{i}—Zn2—O11	99.43 (19)
O5—Zn1—O9^{iii}	89.67 (16)	O6^{i}—Zn2—O8^{ii}	159.08 (17)
O5—Zn1—O1	84.47 (18)	O6^{i}—Zn2—O10	94.97 (17)
O11—Zn2—C1^{ii}	30.0 (2)	O6^{i}—Zn2—C21	104.85 (19)
O8^{ii}—Zn2—O10	81.80 (16)	O6^{i}—Zn2—C1^{ii}	129.3 (2)
O8^{ii}—Zn2—C21	82.22 (17)	O11—Zn2—O9	141.10 (17)
O8^{ii}—Zn2—C1^{ii}	30.22 (19)	O11—Zn2—O8^{ii}	60.25 (16)
O10—Zn2—C21	28.84 (18)	O11—Zn2—O10	92.24 (17)
O10—Zn2—C1^{ii}	86.29 (19)	O11—Zn2—C21	116.37 (19)
C1^{ii}—Zn2—C21	100.1 (2)		

[a]Symmetry codes: (i) −*x*+3/2, *y*−1/2, *z*−1/2; (ii) −*x*+3/2, *y*+1/2, *z*−1/2; (iii) −*x*+3/2, *y*+1/2, *z*+1/2; (iv) −*x*+3/2, *y*−1/2, *z*+1/2; (v) −*x*+1, −*y*+2, *z*+1/2; (vi) −*x*+1, −*y*+2, *z*−1/2.

Table S2: The selected bond distances (Å) and angles (deg) for complex **2**[a].

Zn1—O4	1.975 (3)	Zn2—O3	2.054 (3)
Zn1—O7	2.003 (3)	Zn2—O2	2.004 (3)
Zn1—O5	1.945 (3)	Zn2—O8^{i}	1.998 (3)
Zn1—O9^{i}	1.977 (3)	Zn2—O1	2.121 (3)
Zn1—O6	2.390 (3)	Zn2—O1W	1.960 (3)
O9—Zn1^{ii}	1.977 (3)	O8—Zn2^{ii}	1.998 (3)
O4—Zn1—O7	102.83 (11)	O9^{i}—Zn1—C19	99.05 (14)
O4—Zn1—O9^{i}	94.62 (13)	O6—Zn1—C19	29.18 (12)
O4—Zn1—O6	162.34 (10)	O3—Zn2—O1	171.94 (13)

O4—Zn1—C19	133.33 (13)	O2—Zn2—O3	96.45 (11)
O7—Zn1—O6	59.74 (11)	O2—Zn2—O1	85.44 (12)
O7—Zn1—C19	30.56 (12)	O8^{i}—Zn2—O3	95.00 (12)
O5—Zn1—O4	101.70 (13)	O8^{i}—Zn2—O2	119.93 (12)
O5—Zn1—O7	110.28 (12)	O8^{i}—Zn2—O1	90.80 (14)
O5—Zn1—O9^{i}	133.61 (12)	O1W—Zn2—O3	86.07 (14)
O5—Zn1—O6	88.20 (12)	O1W—Zn2—O2	120.55 (16)
O5—Zn1—C19	100.37 (13)	O1W—Zn2—O8^{i}	118.95 (17)
O9^{i}—Zn1—O7	107.80 (13)	O1W—Zn2—O1	86.23 (15)
O9^{i}—Zn1—O6	88.80 (13)		

[a] Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1; (ii) −*x*+1, *y*+1/2, −*z*+1; (iii) *x*, *y*, *z*−1; (iv) *x*, *y*, *z*+1; (v) *x*−1, *y*, *z*; (vi) *x*+1, *y*, *z*.

Table S3: The selected bond distances (Å) and angles (deg) for complex **3**[a].

Zn1—O1W	1.978 (4)	Zn1—O2^{iii}	2.024 (3)
Zn1—O1^{ii}	2.022 (3)	Zn1—O2^{i}	2.024 (3)
Zn1—O1	2.022 (3)	O2—Zn1^{i}	2.024 (3)
O1W—Zn1—Zn1^{i}	172.60 (18)	O1—Zn1—O2^{iii}	88.59 (17)
O1W—Zn1—O1^{ii}	103.21 (16)	O1^{ii}—Zn1—O2^{iii}	158.71 (15)
O1W—Zn1—O1	103.21 (16)	O1^{ii}—Zn1—O2^{i}	88.59 (17)
O1W—Zn1—O2^{i}	98.06 (17)	O1—Zn1—O2^{i}	158.71 (15)
O1W—Zn1—O2^{iii}	98.06 (16)	O2^{i}—Zn1—Zn1^{i}	76.68 (10)
O1^{ii}—Zn1—Zn1^{i}	82.04 (10)	O2^{iii}—Zn1—Zn1^{i}	76.68 (10)
O1—Zn1—Zn1^{i}	82.04 (10)	O2^{iii}—Zn1—O2^{i}	87.4 (2)
O1—Zn1—O1^{ii}	87.6 (2)		

[a] Symmetry codes: (i) −*x*+5/3, −*y*+4/3, −*z*+4/3; (ii) −*x*+*y*+1, *y*, *z*; (iii) *x*−*y*+2/3, −*y*+4/3, −*z*+4/3; (iv) −*y*+1, −*x*+1, *z*; (v) *y*, *x*, −*z*+1.

2. Ligand

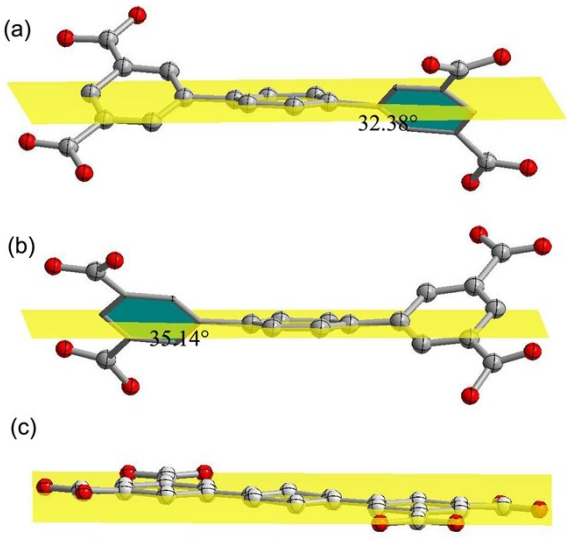

Fig. S1. Linker in the structures of **1-3** (a-c).

2. Powder X-Ray Diffraction

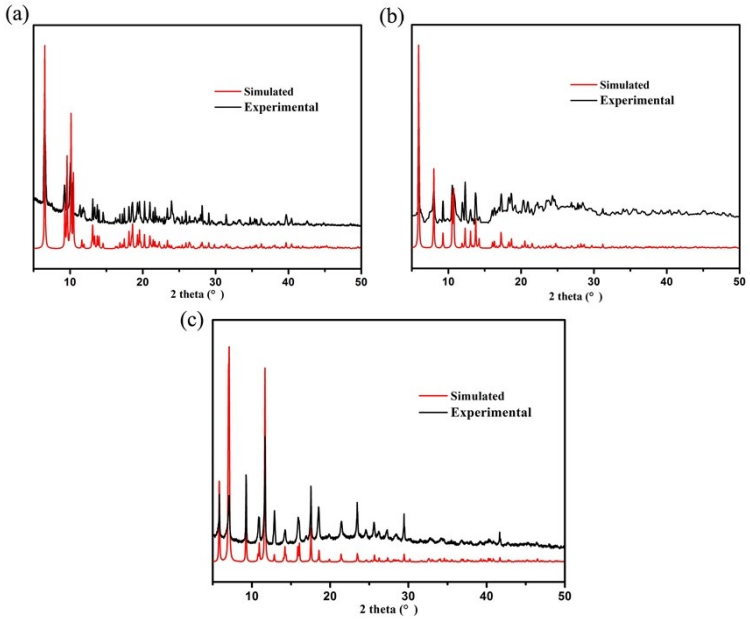

Fig. S2. PXRD patterns of **1-3** (a-c).

3. Thermogravimetric Analysis.

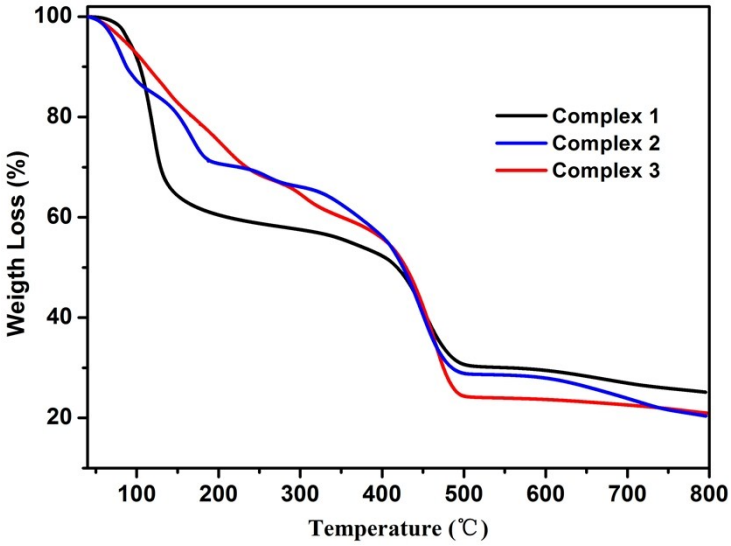

Fig. S3. TGA plots of as-synthesized samples of **1-3** (a-c).

4. Luminescent properties and Fluorescence sensing.

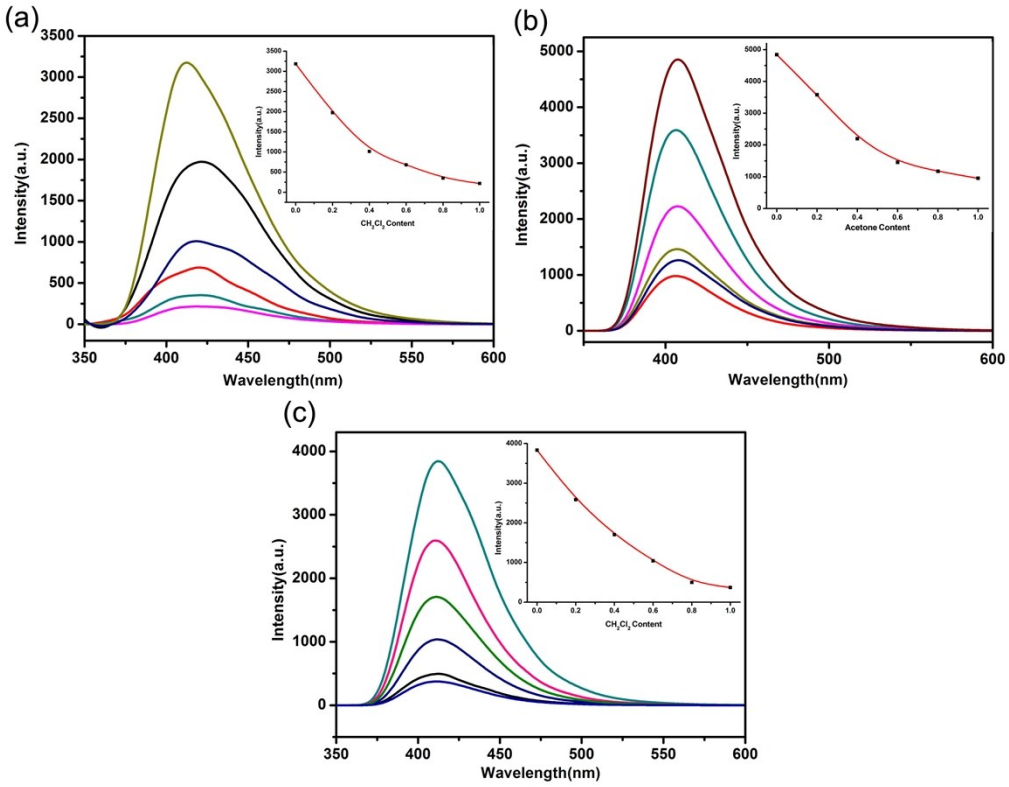

Fig. S4. PL spectra of **1-3** (a-c) that was introduced into two kinds of solvent mixtures with increasing volume of one solvent from 0 to 1 (top-to-bottom). Inset: The PL intensity as a function of volume content. (a) i-PrOH and CH_2Cl_2, (b) CH_3CN and acetone, (c) CH_3CN and CH_2Cl_2

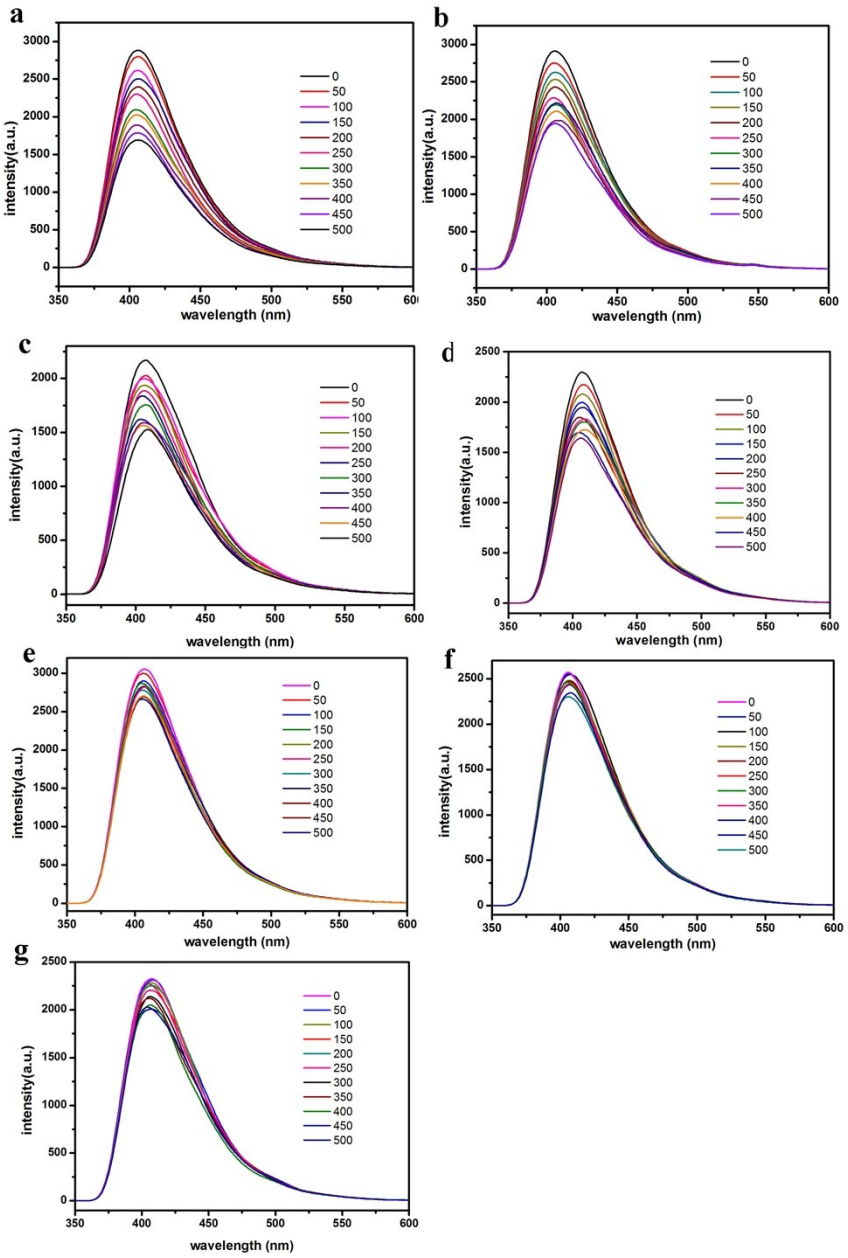

Fig. S5. Effect on the emission spectra of complex **1** dispersed in DMSO upon incremental addition of aromatic compounds solution (1mM) in DMSO, respectively. (1,4-DNB (a), 1,3-DNB (b), 2,4-DNT (c), NT (d), NB (e), CB (f) and BZ (g))

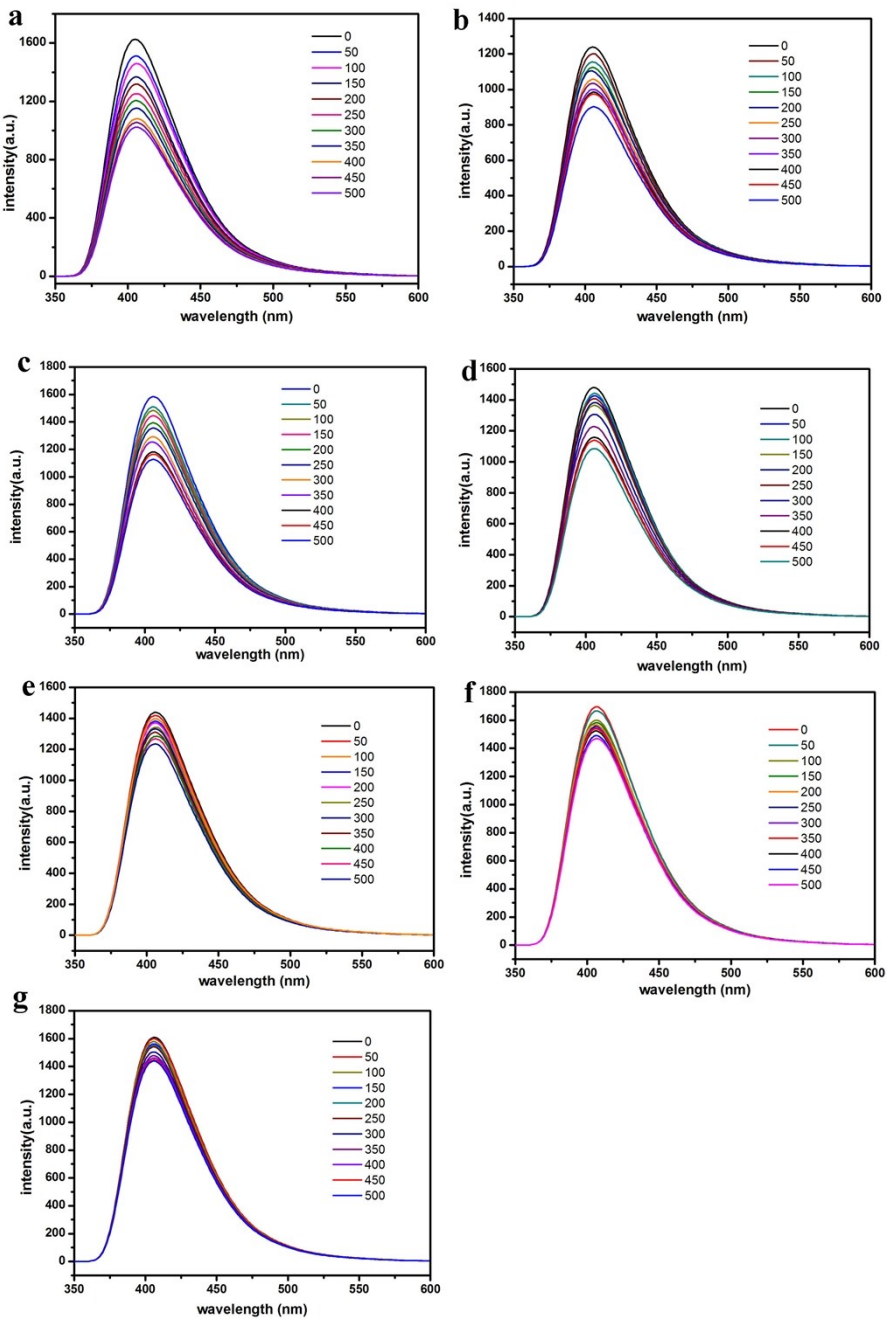

Fig. S6. Effect on the emission spectra of complex **2** dispersed in DMSO upon incremental addition of aromatic compounds solution (1mM) in DMSO, respectively. (1,4-DNB (a), 1,3-DNB (b), 2,4-DNT (c), NT (d), NB (e), CB (f) and BZ (g)).

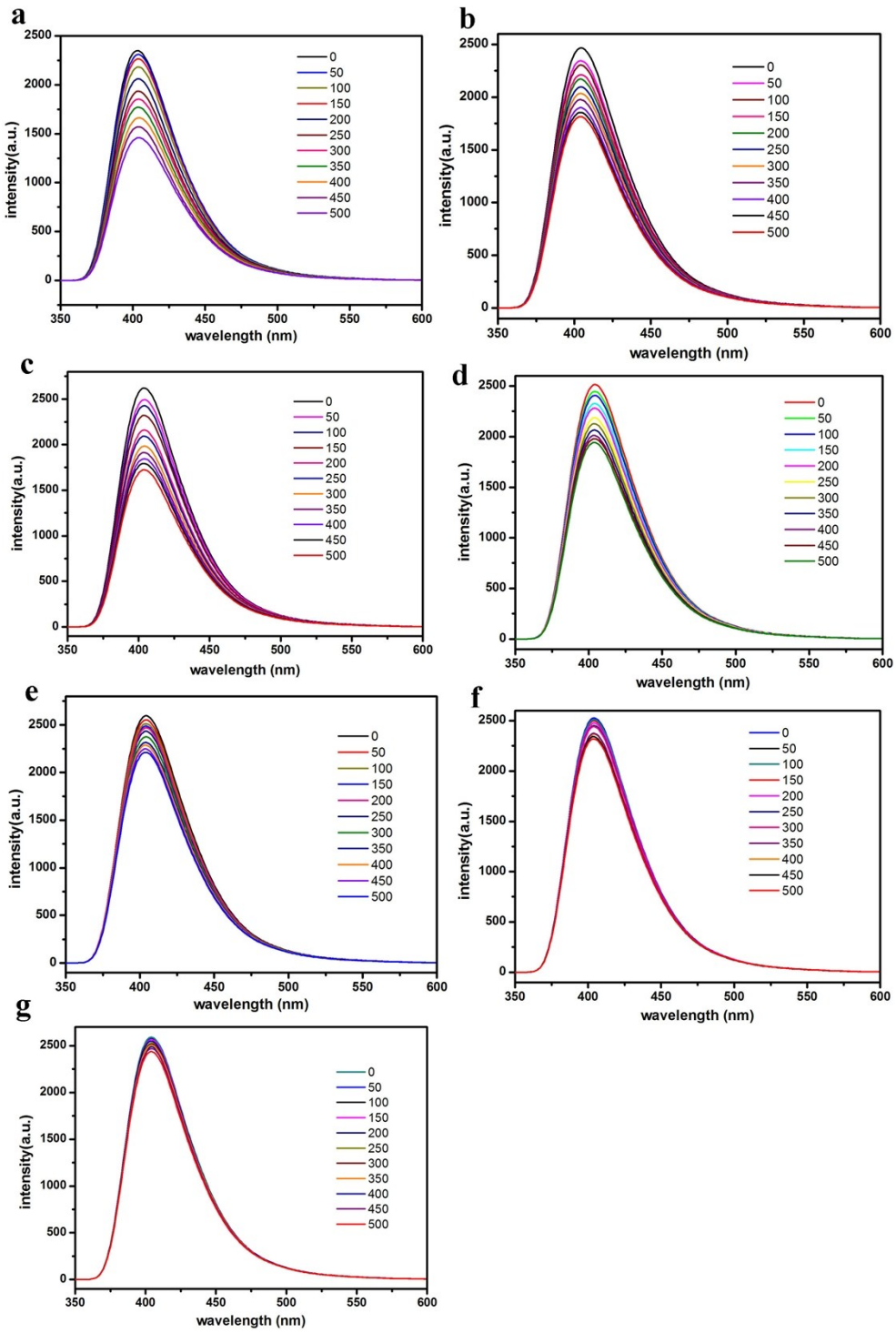

Fig. S7. Effect on the emission spectra of complex **3** dispersed in DMSO upon incremental addition of aromatic compounds solution (1mM) in DMSO, respectively. (1,4-DNB (a), 1,3-DNB (b), 2,4-DNT (c), NT (d), NB (e), CB (f) and BZ (g))

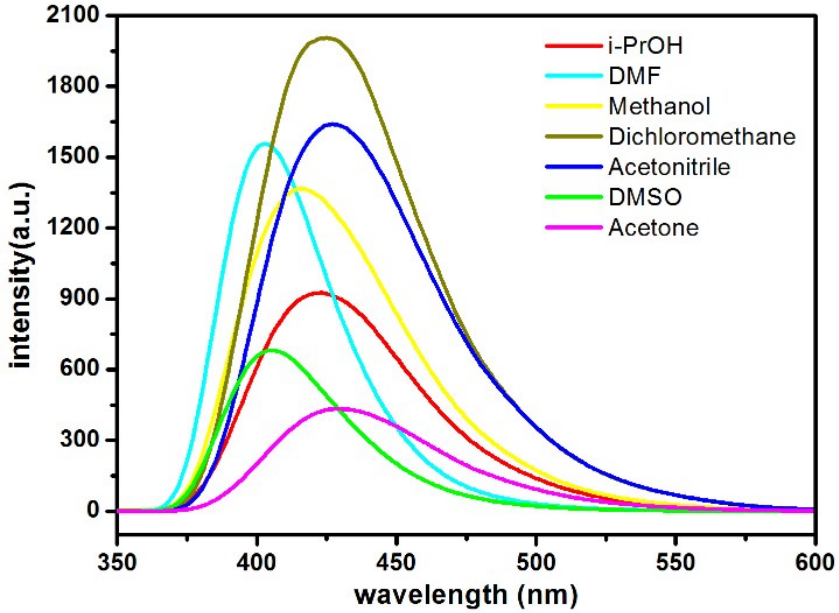

Fig. S8. The photoluminescence spectra of free ligand in various pure solvents