Supplementary Material for Organic & Biomolecular Chemistry

Supporting Information

Synthesis of colorimetric sensors for isomeric dicarboxylate anions: selective discrimination between maleate and fumarate

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This PDF file includes:

Color changes and UV spectra for titration of **1**-**2** with hydroxide. 2D NOESY spectrum of **1** and NMR titration data of **2** with maleate and fumarate.

Figure SI-1a. Color changes of complex **1** upon addition of various anions in DMSO: (a) **1** only; (b) **1**+1.0 equiv. of maleate; (c) **1**+1.0 equiv. of hydroxide.

Figure SI-1b. A family of spectra taken in the course of the titration of a 5×10^{-5} M DMSO solution in **1** with a standard solution of (a) **1**+maleate; (b) **1**+hydroxide

Figure SI-2. NOESY plot of compound **1**

Figure SI-3a. Color changes of complex **2** upon addition of various anions in DMSO: (a) **2** only; (b) **2**+1.0 equiv. of maleate; (c) **2** +1.0 equiv. of hydroxide.

Figure SI-3b. A family of spectra taken in the course of the titration of a 5×10^{-5} M DMSO solution in **2** with a standard solution of (a) **2** +maleate; (b) **2**+hydroxide

Figure SI-4. Partial ^{1}H-NMR spectra of **2** (10 mM) in DMSO-d_6 upon addition of various quantities of maleate：(a) 0 eq; (b) 0.5 eq; (c) 1.0 eq.

Figure SI-5. A family of spectra taken in the course of the titration of a 5×10^{-5} M DMSO solution in **2** with a standard solution of fumarate at 25℃ titration profiles (insert) indicate the formation of a 1:1 complex

Figure SI-6. Partial ^{1}H-NMR spectra of **2** (10 mM) in DMSO-d_6 upon addition of various quantities of fumarate: (a) 0 eq; (b) 0.5 eq; (c) 1.0 eq.

Figure SI-7. A family of spectra taken in the course of the titration of a 5×10^{-5} M DMSO solution in **3** with a standard solution of maleate at 25℃ titration profiles (insert) indicate the formation of a 1:1 complex

Figure SI-8. A family of spectra taken in the course of the titration of a 5×10^{-5} M DMSO solution in **4** with a standard solution of maleate at 25℃ titration profiles (insert) indicate the formation of a 1:1 complex

Figure SI-9. UV-vis spectra changes of **2** operated in DMSO (5×10^{-5} M) after the addition of 2.0 equiv of anions: (a) **2** only, (b) **2**+fumarate, (c) **2**+maleate.

Figure SI-10. UV-vis spectra changes of **3** operated in DMSO (5×10^{-5} M) after the addition of 2.0 equiv of anions: (a) **3** only, (b) **3**+fumarate, (c) **3**+maleate.

Figure SI-11. UV-vis spectra changes of **4** operated in DMSO (5×10^{-5} M) after the addition of 2.0 equiv of anions: (a) **4** only, (b) **4**+fumarate, (c) **4**+maleate.

Figure SI-12. Color changes of complex **1** upon addition of various anions in DMSO : (a) **1** only; (b) **1**+ 2.0 equiv. of *ortho*-phthalate; (c) **1**+ 2.0 equiv. of *meta*-phthalate; (d) **1**+ 2.0 equiv. of *para*-phthalate.

Figure SI-13. Color changes of complex **2** upon addition of various anions in DMSO : (a) **2** only; (b) **2**+ 2.0 equiv. of *ortho*-phthalate; (c) **2**+ 2.0 equiv. of *meta*-phthalate; (d) **2**+ 2.0 equiv. of *para*-phthalate.

Figure SI-14. Color changes of complex **3** upon addition of various anions in DMSO : (a) **3** only; (b) **3**+ 2.0 equiv. of *ortho*-phthalate; (c) **3**+ 2.0 equiv. of *meta*-phthalate; (d) **3**+ 2.0 equiv. of *para*-phthalate.

Figure SI-15. Color changes of complex **4** upon addition of various anions in DMSO : (a) **4** only; (b) **4**+ 2.0 equiv. of *ortho*-phthalate; (c) **4**+ 2.0 equiv. of *meta*-phthalate; (d) **4**+ 2.0 equiv. of *para*-phthalate.

Figure SI-1a. Color changes of complex **1** upon addition of various anions in DMSO :(a) **1** only; (b) **1**+1.0 equiv. of maleate; (c) **1**+1.0 equiv. of hydroxide.

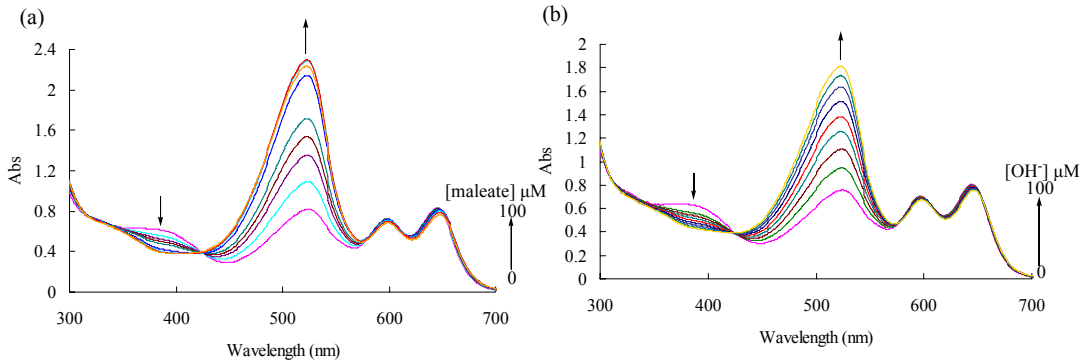

Figure SI-1b. A family of spectra taken in the course of the titration of a 5×10^{-5} M DMSO solution in **1** with a standard solution of (a) **1**+maleate; (b) **1**+hydroxide

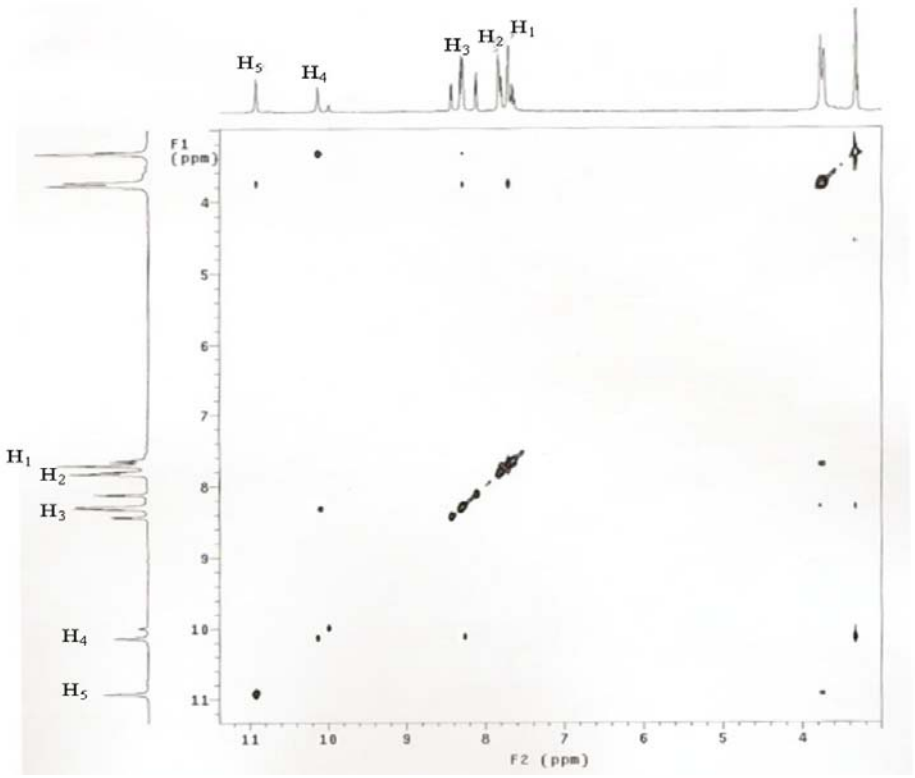

Figure SI-2. NOESY plot of compound **1**

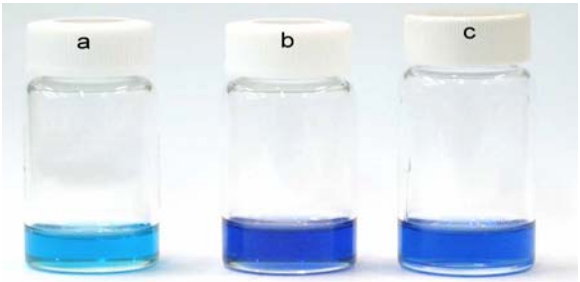

Figure SI-3a. Color changes of complex **2** upon addition of various anions in DMSO :(a) **2** only; (b) **2**+1.0 equiv. of maleate; (c) **2**+1.0 equiv. of hydroxide.

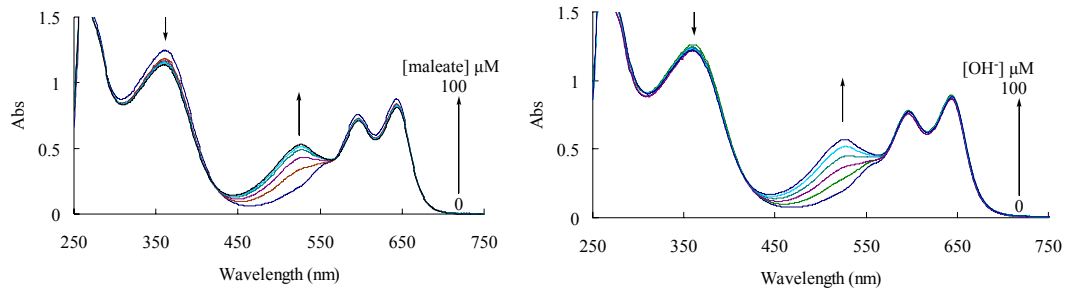

Figure SI-3b. A family of spectra taken in the course of the titration of a 5×10^{-5} M DMSO solution in **2** with a standard solution of (a) **2**+maleate; (b) **2**+hydroxide.

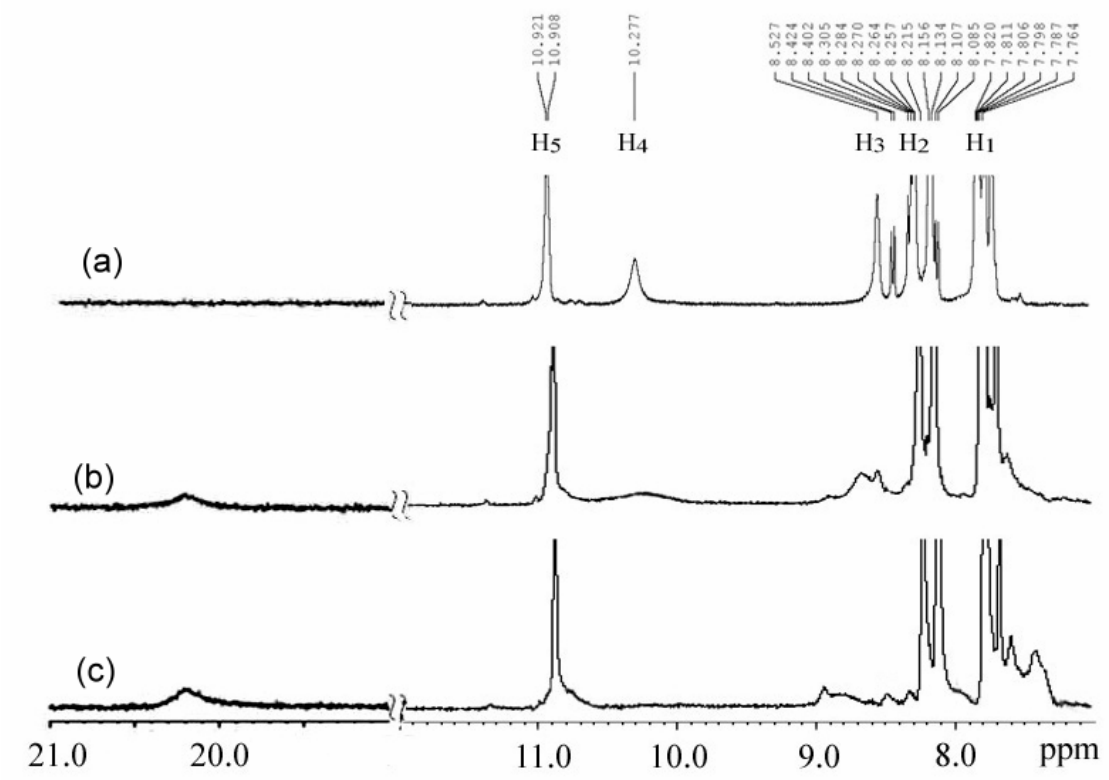

Figure SI-4. Partial ^{1}H-NMR spectra of **2** (10 mM) in DMSO-d_6 upon addition of various quantities of maleate：(a) 0 eq; (b) 0.5 eq; (c) 1.0 eq.

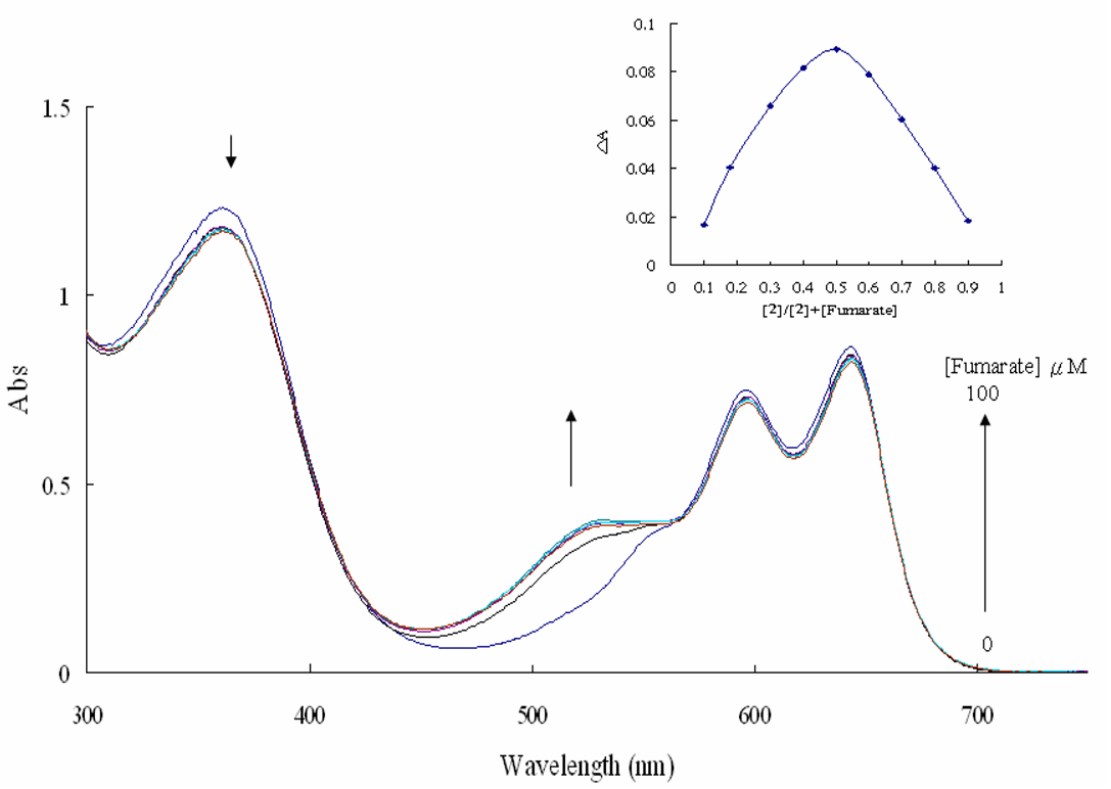

Figure SI-5. A family of spectra taken in the course of the titration of a 5×10^{-5} M DMSO solution in **2** with a standard solution of fumarate at 25℃ titration profiles (insert) indicate the formation of a 1:1 complex

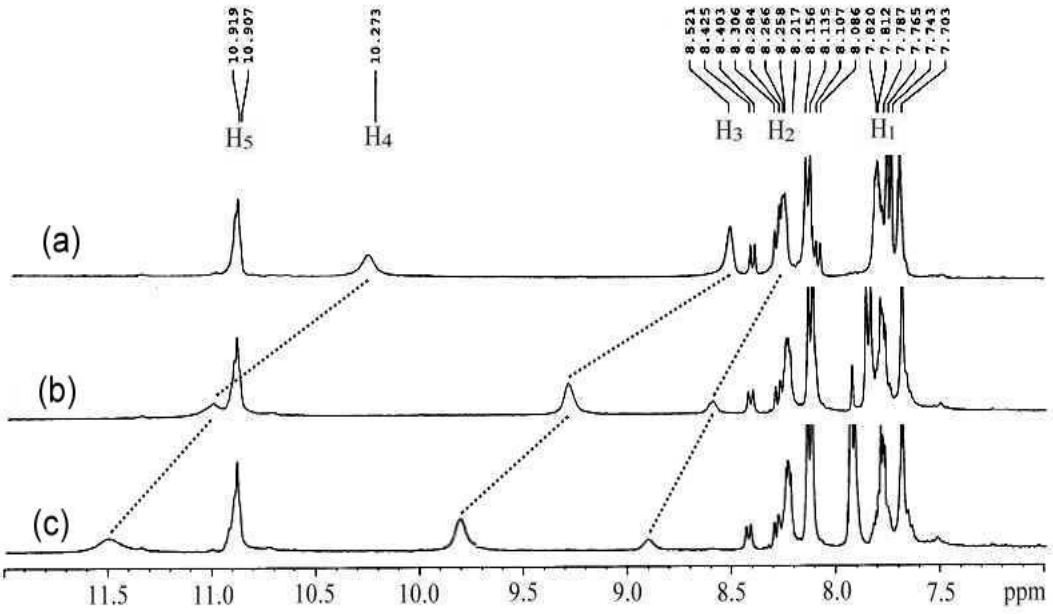

Figure SI-6. Partial ^{1}H-NMR spectra of **2** (10 mM) in DMSO-d_6 upon addition of various quantities of fumarate：(a) 0 eq; (b) 0.5 eq; (c) 1.0 eq.

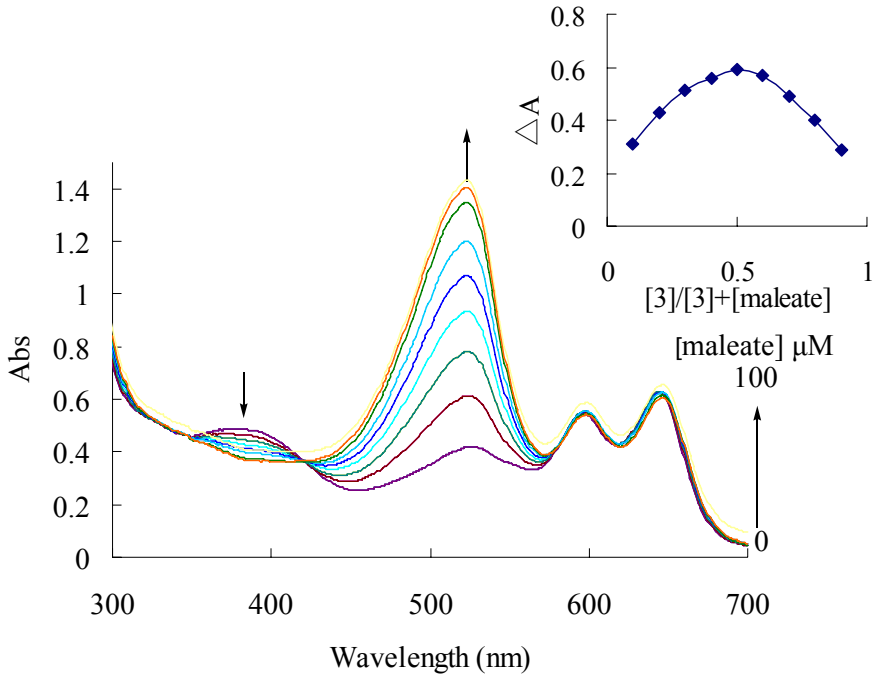

Figure SI-7. A family of spectra traken in the course of the titration of a 5×10^{-5} M DMSO solution in **3** with a standard solution of maleate at 25℃ titration profiles (insert) indicate the formation of a 1：1 complex.

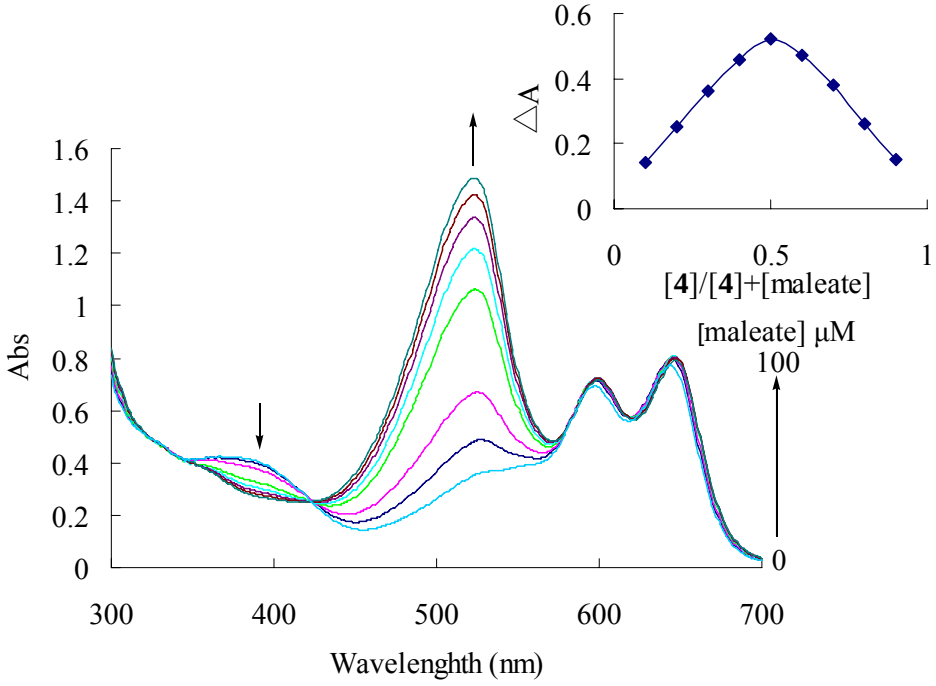

Figure SI-8. A family of spectra taken in the course of the titration of a 5×10^{-5} M DMSO solution in **4** with a standard solution of maleate at 25℃ tration profiles (insert) indicate the formation of a 1:1 complex.

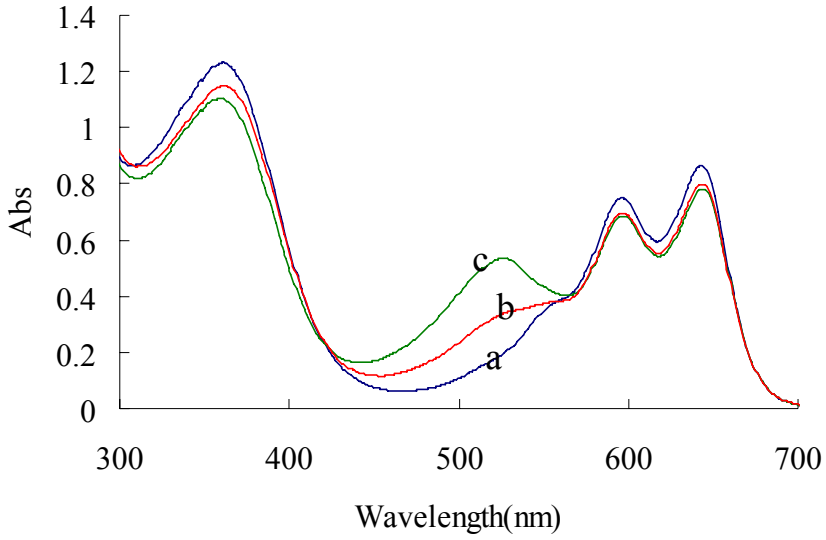

Figure SI-9. UV-vis spectra changes of **2** operated in DMSO (5×10^{-5} M) after the addition of 2.0 equiv of anions: (a) **2** only, (b) **2**+fumarate, (c) **2**+maleate.

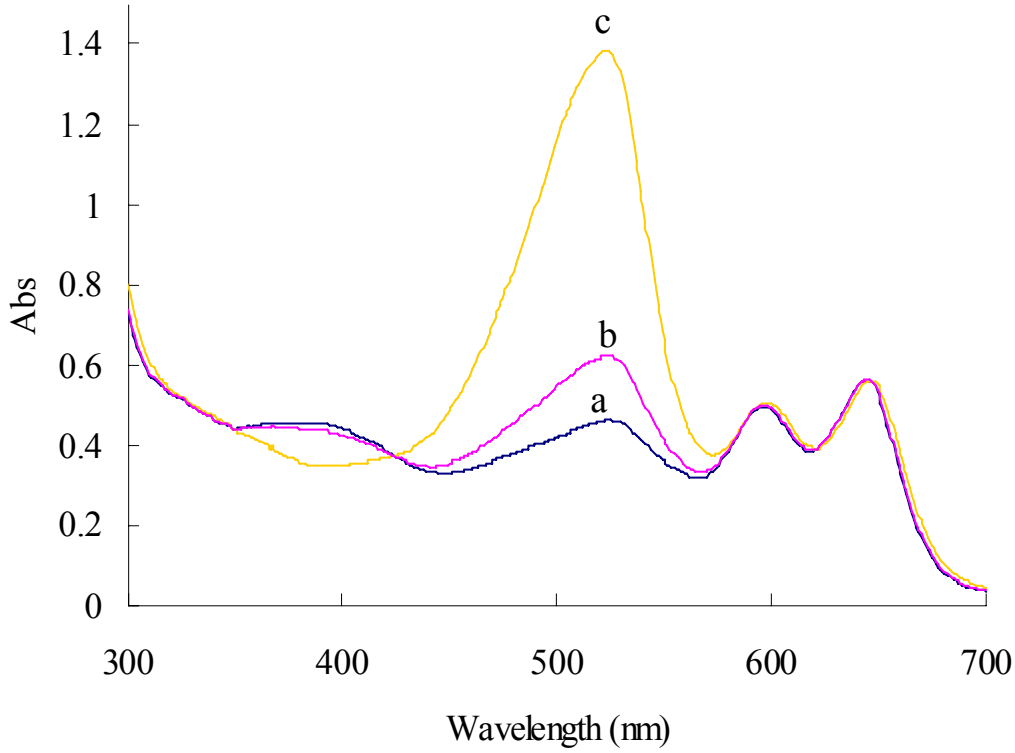

Figure SI-10. UV-vis spectra changes of **3** operated in DMSO (5×10^{-5} M) after the addition of 2.0 equiv of anions: (a) **3** only, (b) **3**+fumarate, (c) **3**+maleate

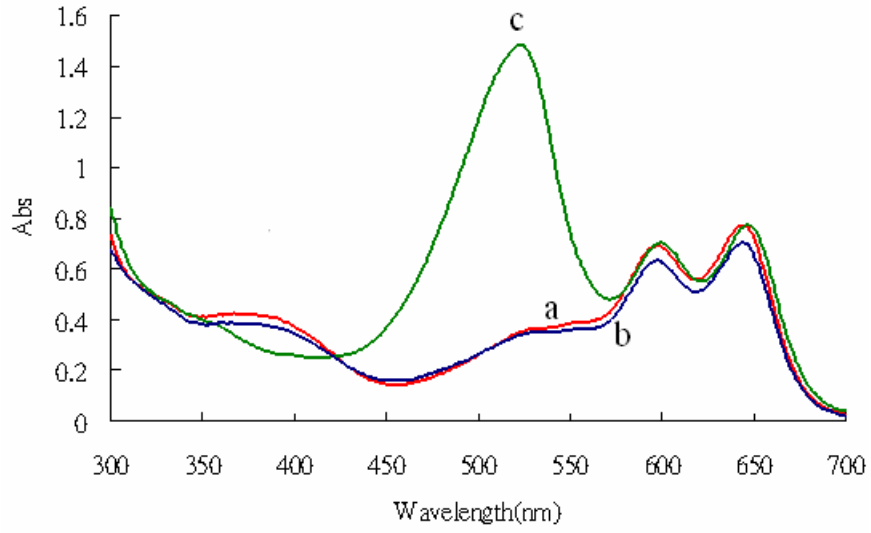

Figure SI-11. UV-vis spectra changes of **4** operated in DMSO (5×10^{-5} M) after the addition of 2.0 equiv of anions: (a) **4** only, (b) **4**+ fumarate, (c) **4**+ maleate

Figure SI-12. Color changes of complex **1** upon addition of various anions in DMSO : (a) **1** only; (b) **1**+ 2.0 equiv. of *ortho*-phthalate; (c) **1**+ 2.0 equiv. of *meta*-phthalate; (d) **1**+ 2.0 equiv. of *para*-phthalate.

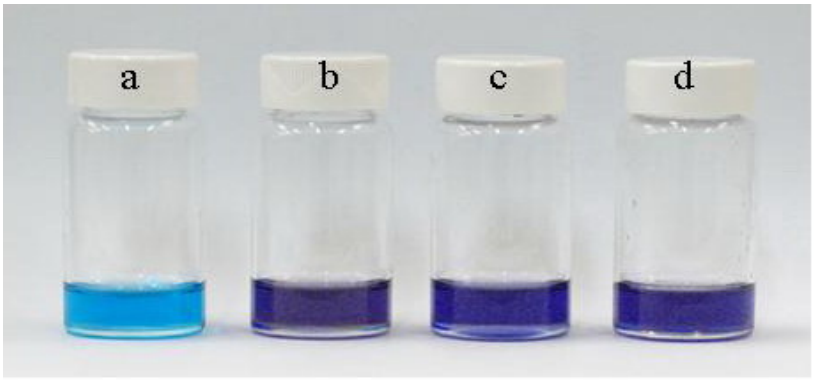

Figure SI-13. Color changes of complex **2** upon addition of various anions in DMSO : (a) **2** only; (b) **2**+ 2.0 equiv. of *ortho*-phthalate; (c) **2**+ 2.0 equiv. of *meta*-phthalate; (d) **2**+ 2.0 equiv. of *para*-phthalate.

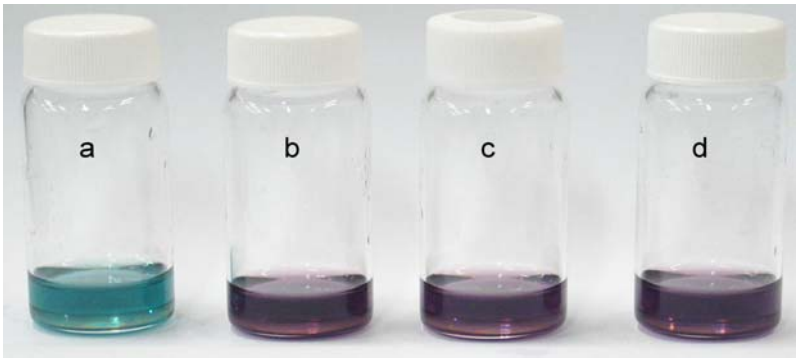

Figure SI-14. Color changes of complex **3** upon addition of various anions in DMSO : (a) **3** only; (b) **3**+ 2.0 equiv. of *ortho*-phthalate; (c) **3**+ 2.0 equiv. of *meta*-phthalate; (d) **3**+ 2.0 equiv. of *para*-phthalate.

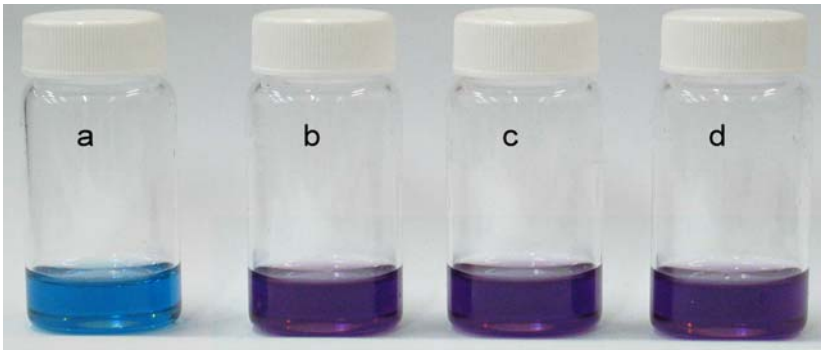

Figure SI-15. Color changes of complex **4** upon addition of various anions in DMSO : (a) **4** only; (b) **4**+ 2.0 equiv. of *ortho*-phthalate; (c) **4**+ 2.0 equiv. of *meta*-phthalate; (d) **4**+ 2.0 equiv. of *para*-phthalate.