Electronic Supplementary Information

A pyrophosphate-induced reorganization of reporter-receptor assembly via boronate esterification; new strategy of a turn-on fluorescent detection of multi-phosphates in aqueous solution

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1. PPi-induced fluorescence enhancement

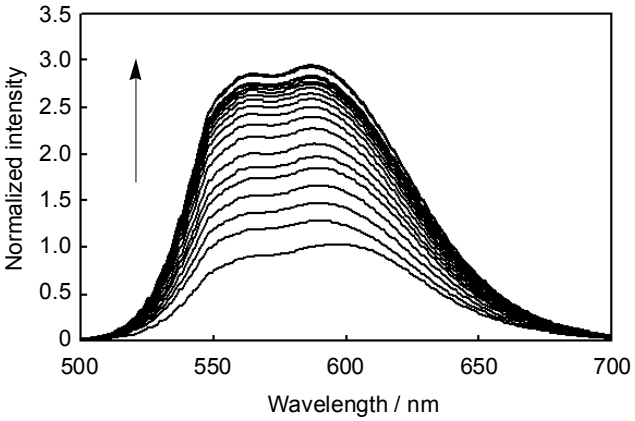


Fig. S1. Change in fluorescence spectra (λ_{ex} = 480 nm) for ARS (50 μM) upon addition of PPi (0 – 500 μM) in the presence of **1·Zn** (250 μM) in MeOH-10 mM HEPES buffer (1:1 v/v) containing 10 mM NaCl at pH 7.4 at 25 ºC.

2. Fluorescence spectrum of ARS with Zn^{II}-DPA-free phenylboronic acid

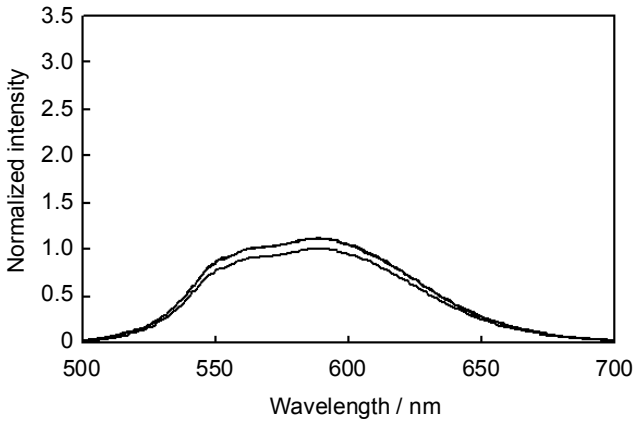


Fig. S2. Change in fluorescence spectra (λ_{ex} = 480 nm) for ARS (50 μM) upon addition of PPi (0 – 1000 μM) in the presence of phenylboronic acid (250 μM) in MeOH-10 mM HEPES buffer (1:1 v/v) containing 10 mM NaCl at pH 7.4 at 25 ºC.

3. ^{1}H, ^{1}H COSY spectrum of alizarin plus 1·Zn with PPi

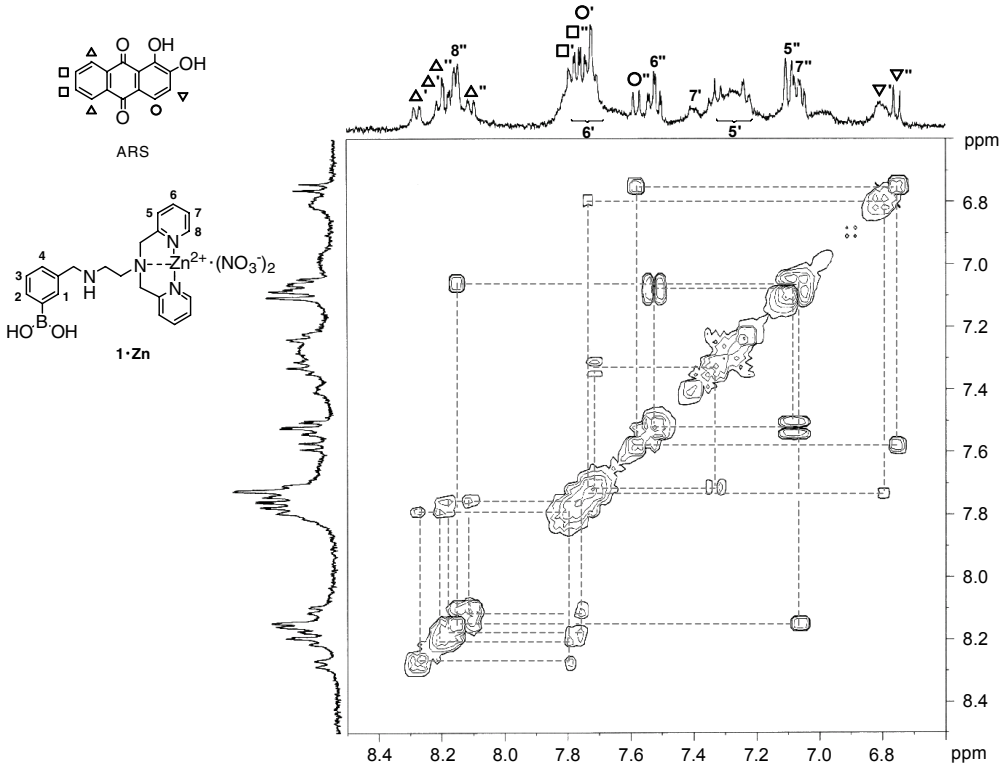
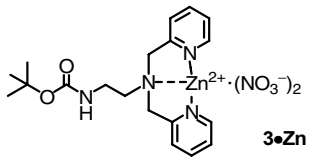


Fig. S3. ^{1}H, ^{1}H COSY spectrum in CD_3OD–D_2O (9:1 v/v) (400 MHz, r.t.). [alizarin] = 2.4 mM, [**1·Zn**] = 2.4 mM. The spectrum was obtained after (solid (PPi) – liquid (2.4 mM of alizarin and **1·Zn** in CD_3OD–D_2O (9:1 v/v)) two-phase extraction.

3. Fluorescence spectra of ARS upon adding an incremental amount of 3·Zn



3•Zn

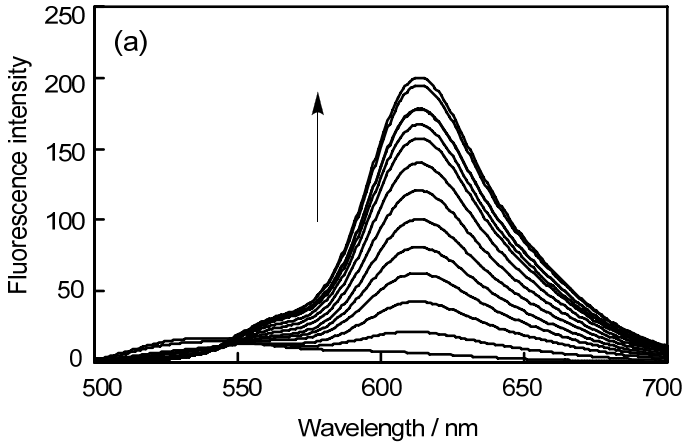


Fig. S4. The fluorescence spectra for ARS (50 μM) upon addition of **3·Zn** (0 – 250 μM) in MeOH-10 mM HEPES buffer (1:1 v/v) containing 10 mM NaCl at pH 7.4 at 25 ºC, λ_{ex} = 480 nm.