Electronic Supporting Information:

Studies on acedan-based mononuclear zinc complexes toward selective fluorescent probes for pyrophosphate

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Fig. S1 $^1$H NMR (300 MHz) spectral change of 3 (10 mM) upon addition of Zn$^{2+}$ (4 $\times$ 2.5 mM) in CD$_3$CN.
Fig. S2 Isothermal Titration Calorimetry (ITC) data: (a) 3 (0.2 mM) with Zn(ClO₄)₂ (3.0 mM); measured in CH₃CN at 30 °C.

Procedure: To a solution of 3 in the calorimeter cell, 5.0 μL of zinc perchlorate was injected 40 times at 30 °C. The dilution effects were corrected by carrying out a separate blank titration. The titration data was analyzed by the built-in curve-fitting Origin software: the “two sets of sites” model was used, which applies to a receptor system that has non-identical and independent sites for binding (support@microcalorimetry.com).

Conditions:
Cell: 3 (0.2 mM) in acetonitrile
Syringe: zinc perchlorate hexahydrate solution (3.0 mM) in acetonitrile
Reference power: 26
Temperature: 30 °C
Stirring rate: 220 rpm.
Fig. S3 HRMS (FAB+) of 3-Zn(II) as perchlorate salt.
Fig. S4 UV absorption changes of (a) 3, (b) 4a and (c) 4b (10 µM each) with addition of Zn²⁺ (1 equiv.) in HEPES buffer (10 mM, pH 7.4; containing 1% CH₃CN) followed by anion (1 equiv.) addition. PPI, ATP, ADP, and AMP were used as corresponding sodium salts.
**Fig. S5** Fluorescence spectral change of 3 (10 µM) upon addition of Zn$^{2+}$ (1 equiv.) in pH 7.4 buffer (10 mM HEPES containing 1% CH$_3$CN). $\lambda_{ex} = 295$ nm. Due to second-order diffraction interference fluorescence data were cut down at 570 nm.

**Fig. S6** Fluorescence spectral change of 3-Zn (10 µM) upon addition of PPi (top) and ATP (bottom) up to 20 µM in pH 7.4 buffer (10 mM HEPES containing 1% CH$_3$CN). $\lambda_{ex} = 295$ nm. Inset is a part of the plot in the range from 0 to 0.5 µM. Due to second-order diffraction interference fluorescence data were cut down at 550 nm.