Supporting Information for

A cholic acid-based fluorescent chemosenor for the detection of ATP

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1. UV titration of the control compound 1b with four nucleobases

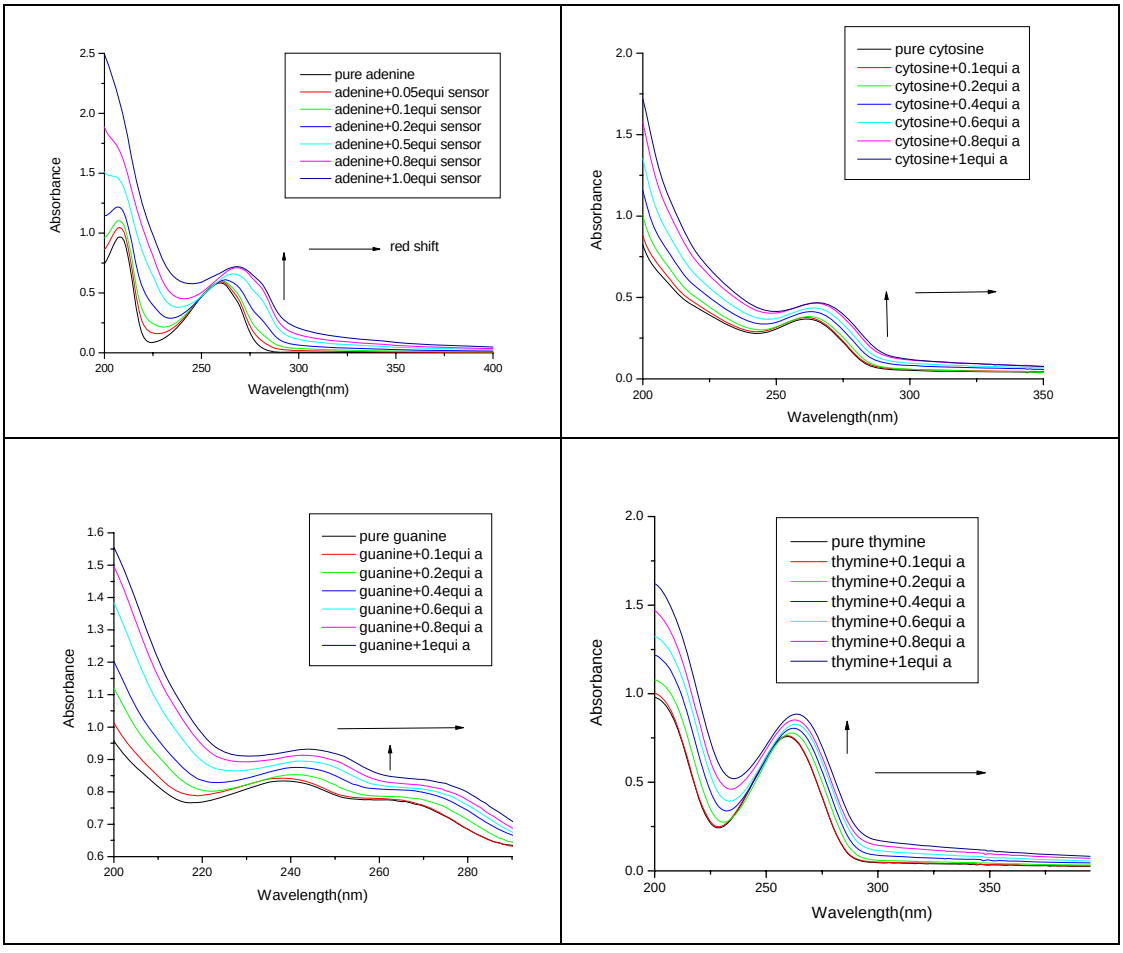

Fig. S1 Change in absorbance for adenine base (C, G, T) (50 μM) upon addition of compound **4** in CH_3CN:H_2O=1:1, HEPES=10mM, pH=7.4.

	$(A-A_0)/A_0$	Red shift
A	38.7%	8nm
C	27.3%	5nm
G	16.7%	5nm
T	11.5%	5nm

2. Job plot of 1a with sodium salt of ATP

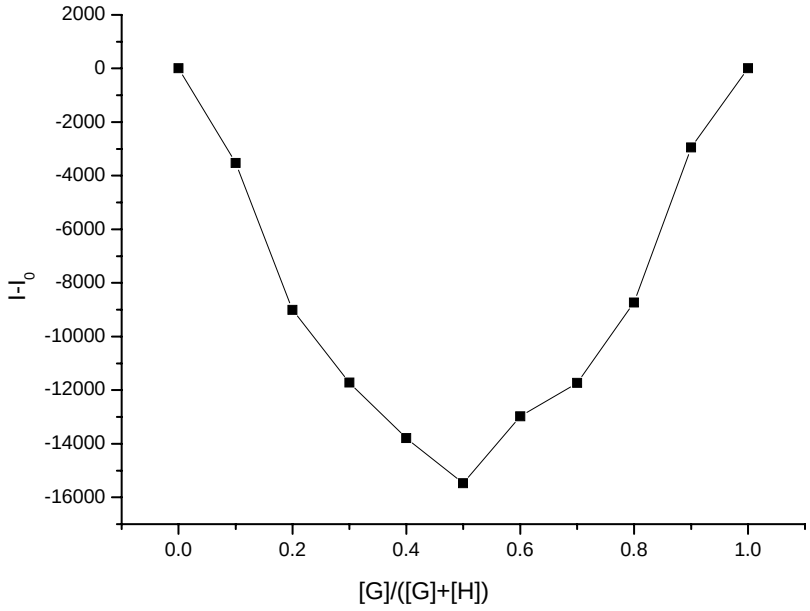

FIG S2. Job's plot of sensor with sodium salt of ATP in $CH_3CN:H_2O$=1:1, HEPES=10mM, pH=7.4.

3. **Table S1** Solvent effect on the binding of **1a** and ATP

$CH_3CN:H_2O$	**Binding constant K_{ass} (M^{-1})**	**R**
2:8	$(9.73 \pm 0.43) \times 10^5$	0.9904
4:6	$(3.16 \pm 0.18) \times 10^6$	0.9940
5:5	$(6.95 \pm 0.11) \times 10^6$	0.9962
6:4	$(9.11\pm 0.65) \times 10^6$	0.9927
8:2	$(1.84\pm 0.32) \times 10^7$	0.9913

4. ^{13}C NMR data of the binding experiment

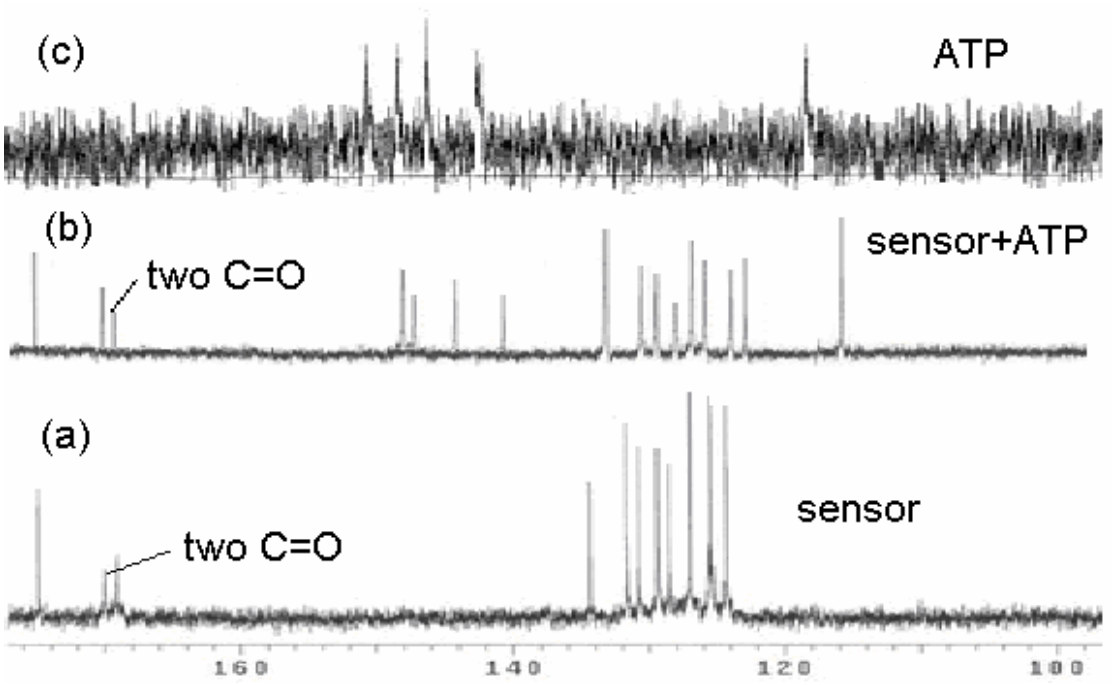

Fig. S3 Partial ^{13}C NMR spectra of (a) sensor, (b) sensor + ATP (1 equiv) and (c) ATP in CD_3CN: D_2O=1:1.

Adenine

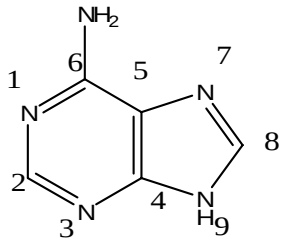

Table S2 Chemical induced shift of selected carbons of ATP triggered by the complexation

Carbons	C-2	C-4	C-5	C-6	C-8
Adenine	152.5	151.4	117.6	155.4	139.4
ATP	148.4	146.0	118.5	150.4	142.5
ATP-sensor	147.2	144.6	116.3	147.6	141.2
CIS (ppm)	-1.2	-1.4	-2.2	-2.8	-1.3