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(Supporting Information)

Thermally prepared ultrabright adenosine monophosphate capped gold nanoclusters and the intrinsic mechanism

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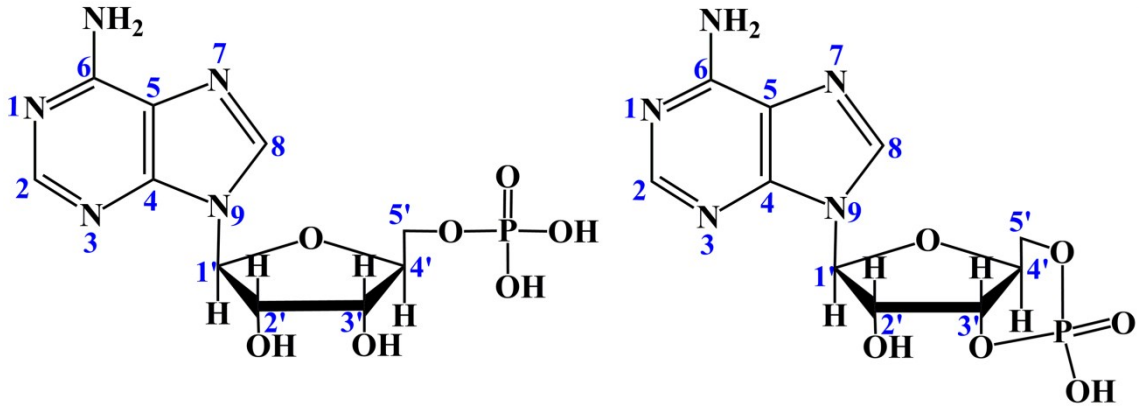

Scheme S1. The schematic structure and atom sequence of adenosine5'-monophosphate (AMP, left) and adenosine 3',5'-cyclic monophosphate (cAMP, right), respectively.

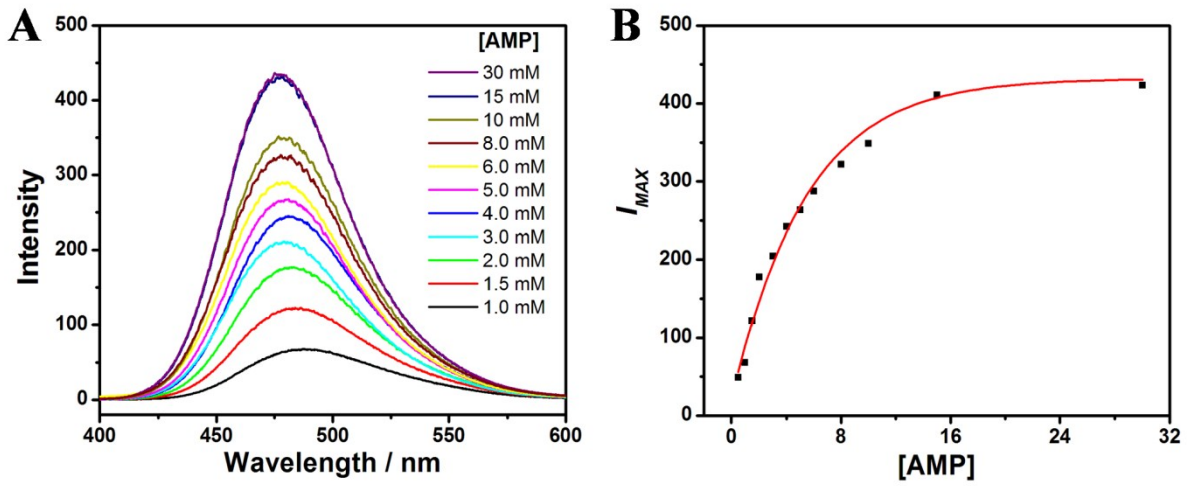

Fig. S1 (A) The fluorescence spectra of AuNCs@AMP prepared in the presence of different amount of AMP, where the initial concentrations of $HAuCl_4$ and citrate were kept at 1.0 and 50 mM, respectively; (B) The corresponding maximum intensities in changing with the amount of AMP (λ_{ex} = 328 nm).

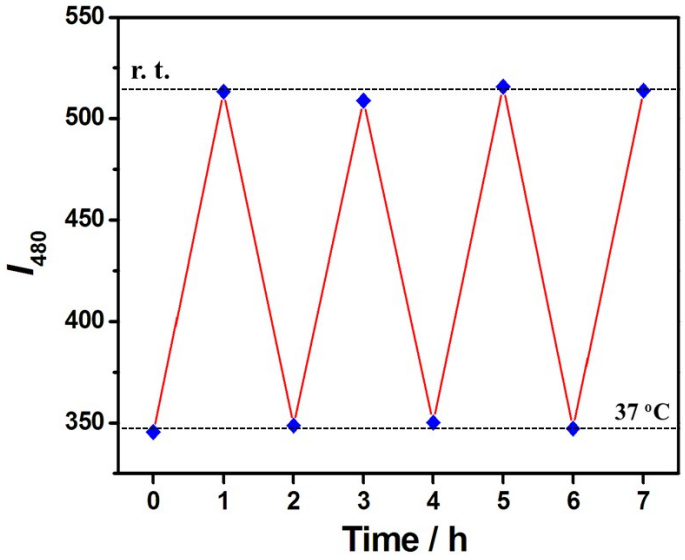

Fig. S2 The fluorescence stability of AuNCs@AMP (3.0 mg/L) in phosphate buffer solution (20 mM, pH = 7.4), being incubated at 37 °C and room temperature (r. t.), respectively, for several circulatory.

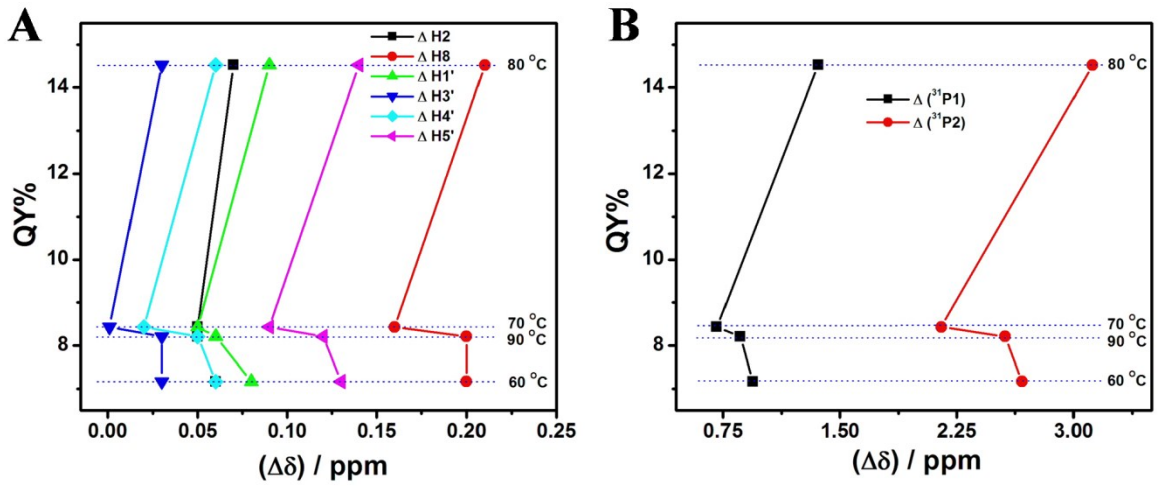

Fig. S3 The connection of QY and chemical shift changes of (A) each proton in ^{1}H NMR and (B) phosphate in ^{31}P NMR spectrum of AuNCs@AMP.

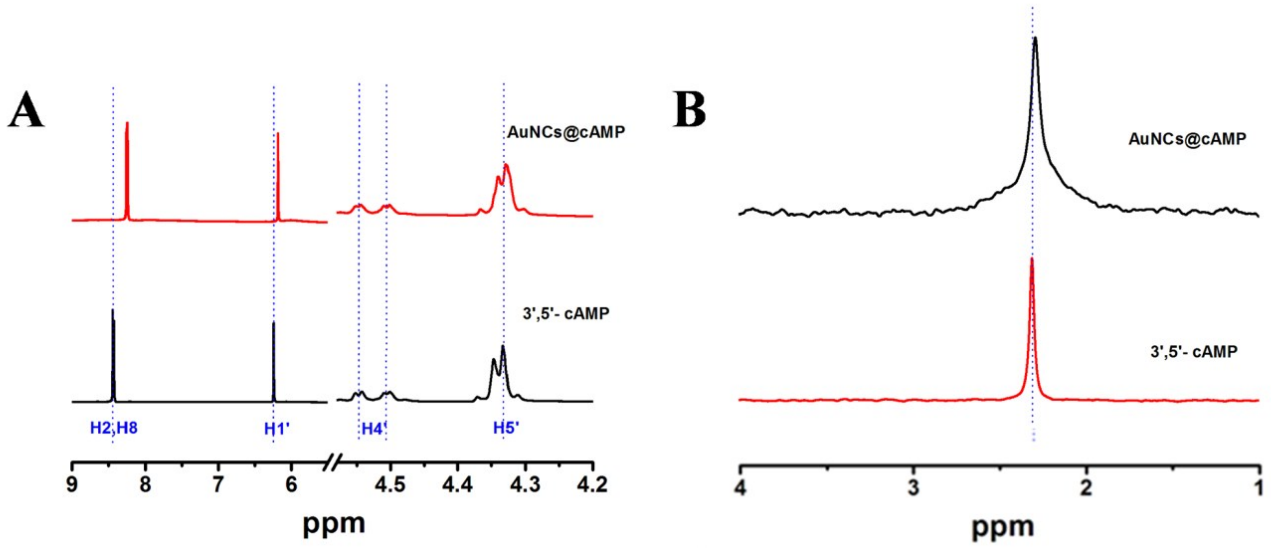

Fig. S4 (A) ^{1}H and (B) ^{31}P NMR spectra (D_2O 10%) of cAMP and the AuNCs@cAMP prepared at 80 °C.

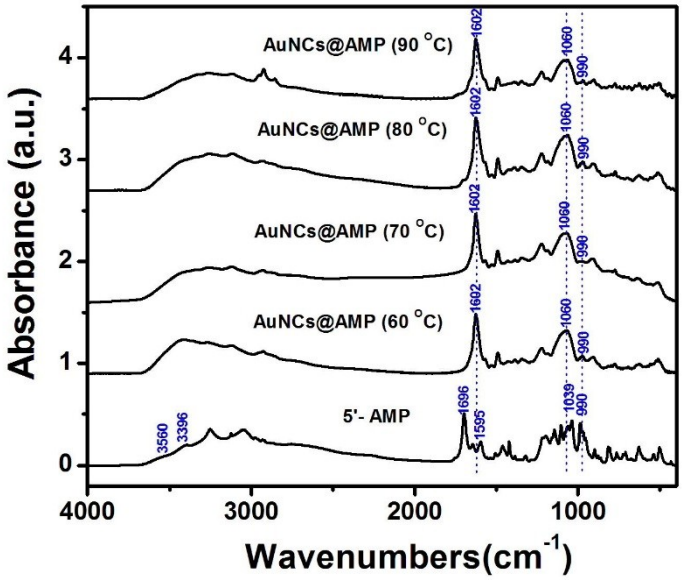

Fig. S5 FT-IR spectra of AMP and AuNCs@AMP prepared at 60, 70, 80 and 90 °C, respectively, dispersed in KBr pellet in the region of 4000-400 cm^{-1}.

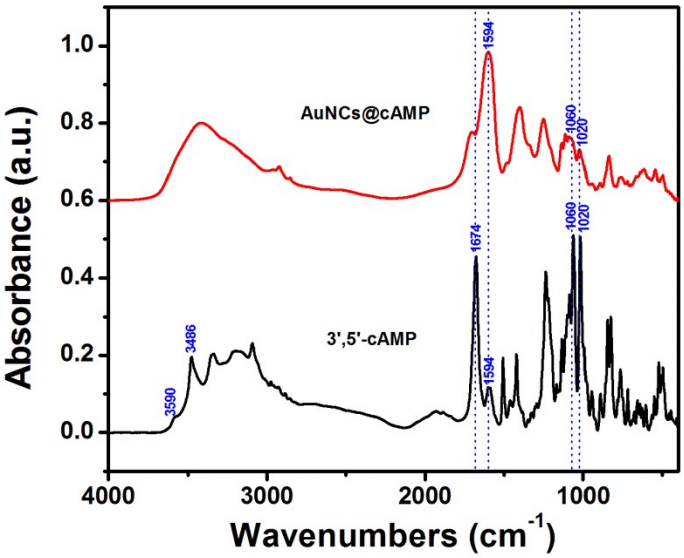

Fig. S6 FT-IR spectra of cAMP and $AuNC_S$@cAMP dispersed in KBr pellet in the region of 4000-400 cm^{-1}.

Table S1 The relative QY of AuNCs@AMP prepared at different temperature with ligand of AMP or cAMP.

Samples	AuNCs@AMP (60 °C)	AuNCs@AMP (70 °C)	AuNCs@AMP (80 °C)	AuNCs@AMP (90 °C)	AuNCs@cAMP (70 °C)	AuNCs@cAMP (80 °C)
QY	7.17%	8.43%	14.52%	8.21%	14.03%	15.33%

Table S2 The relative changes of chemical shifts for each proton in AuNCs@AMP from AMP.

Chmical shift	5'-AMP	AuNCs@AMP (60 °C)		AuNCs@AMP (70 °C)		AuNCs@AMP (80 °C)		AuNCs@AMP (90 °C)	
(ppm)	δ_0	δ	Δ δ	δ	Δ δ	δ	Δ δ	δ	Δ δ
H2	8.63	8.57	-0.06	8.58	-0.05	8.56	-0.07	8.58	-0.05
H8	8.45	8.25	-0.20	8.29	-0.16	8.24	-0.21	8.25	-0.02
H1'	6.20	6.12	-0.08	6.15	-0.05	6.11	-0.09	6.14	-0.06
H3'	4.52	4.49	-0.03	4.52	0	4.50	-0.02	4.49	-0.03
H4'	4.41	4.35	-0.06	4.39	-0.02	4.35	-0.06	4.36	-0.05
H5'	4.16	4.03	-0.13	4.07	-0.09	4.01	-0.14	4.04	-0.12

Table S3 The changes of chemical shift of ^{31}P in AuNCs@AMP in comparison to that of AMP.

Chemical shift	5'-AMP	AuNCs@AMP (60 °C)		AuNCs@AMP (70 °C)		AuNCs@AMP (80 °C)		AuNCs@AMP (90 °C)	
(ppm)	δ_0	δ	Δ δ	δ	Δ δ	δ	Δ δ	δ	Δ δ
^{31}P	4.18	5.12	0.94	4.89	0.71	5.54	1.36	5.04	0.86
		6.85	2.67	6.33	2.15	7.30	3.12	6.74	2.56

Table S4 Comparison of the typical intensity ratios of AMP and AuNCs@AMP, cAMP and AuNCs@cAMP, respectively.

Intensity ratio	5'-AMP	AuNCs@AMP (60 °C)	AuNCs@AMP (70 °C)	AuNCs@AMP (80 °C)	AuNCs@AMP (90 °C)	3',5'-cAMP	AuNCs@cAMP (80 °C)
I_{990}/I_{1060}	0.98	0.39	0.38	0.53	0.43	–	–
I_{1602}/I_{1696}	0.40	1.24	1.35	1.48	1.13	0.23	3.9