Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Unravelling Molecular Interaction of Uranyl(VI) Complex with Bovine Serum Albumin

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Electronic Supplementary Information

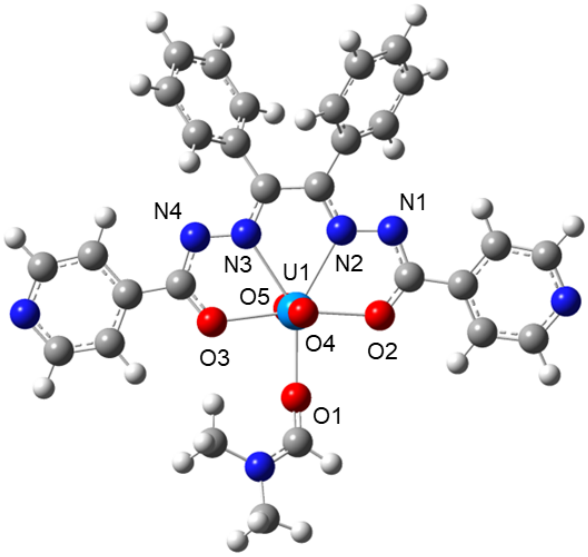

Fig. S1 Energy optimized structure of UC.

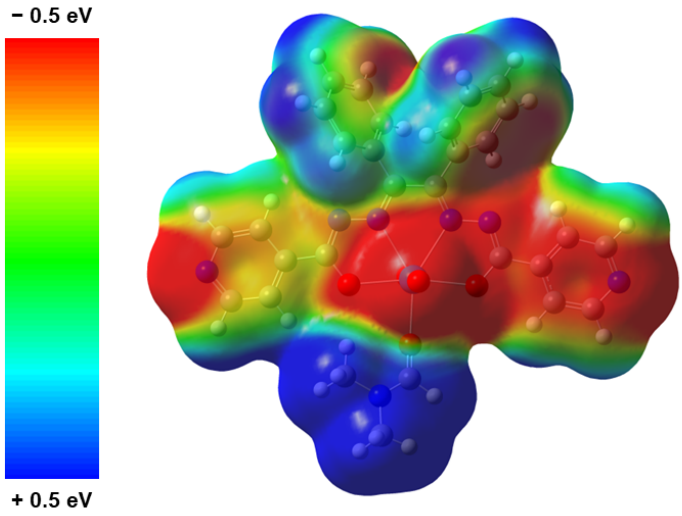

Fig. S2 Molecular electrostatic potential surface of UC.

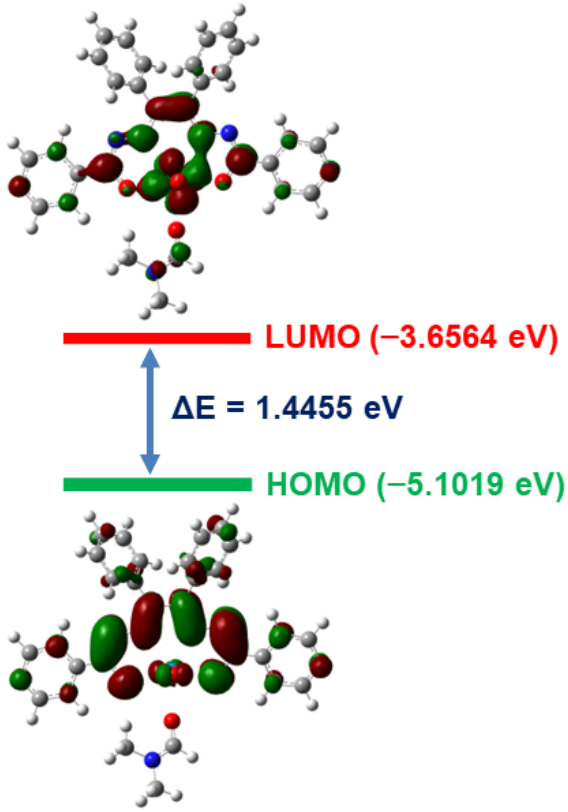

Fig. S3 HOMO−LUMO energy level diagram of UC.

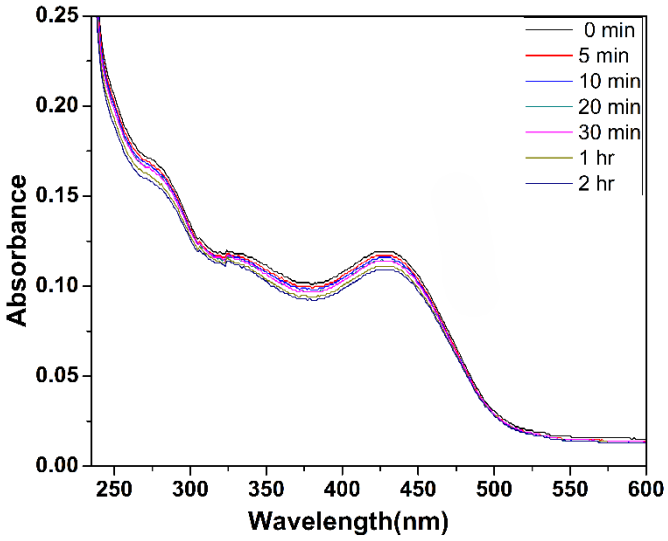

Fig. S4 UV-vis spectra of UC (1.0×10^{-4} M) in PBS at different time intervals.

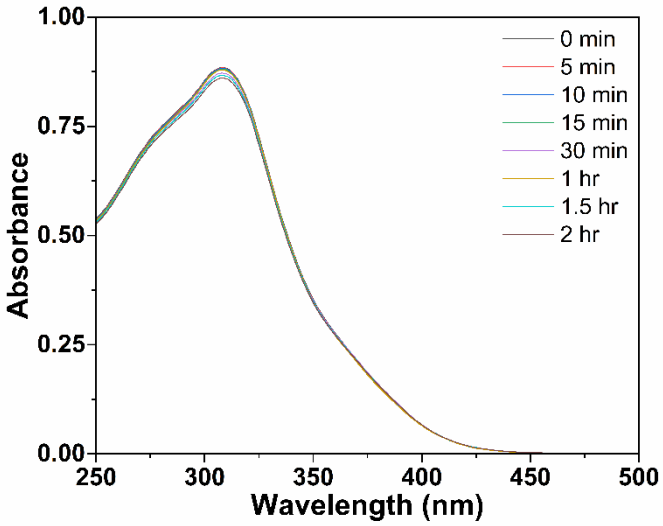

Fig. S5 UV-vis spectra of H_2L (1.0×10^{-4} M) in PBS at different time intervals.

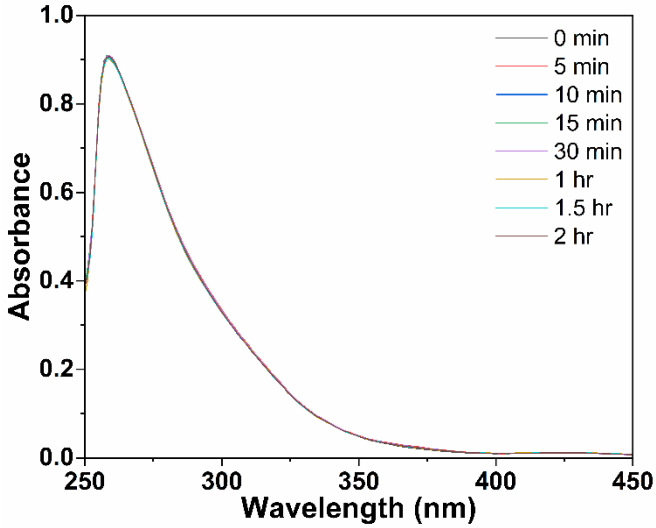

Fig. S6 UV-vis spectra of UA (1.0×10^{-4} M) in PBS at different time intervals.

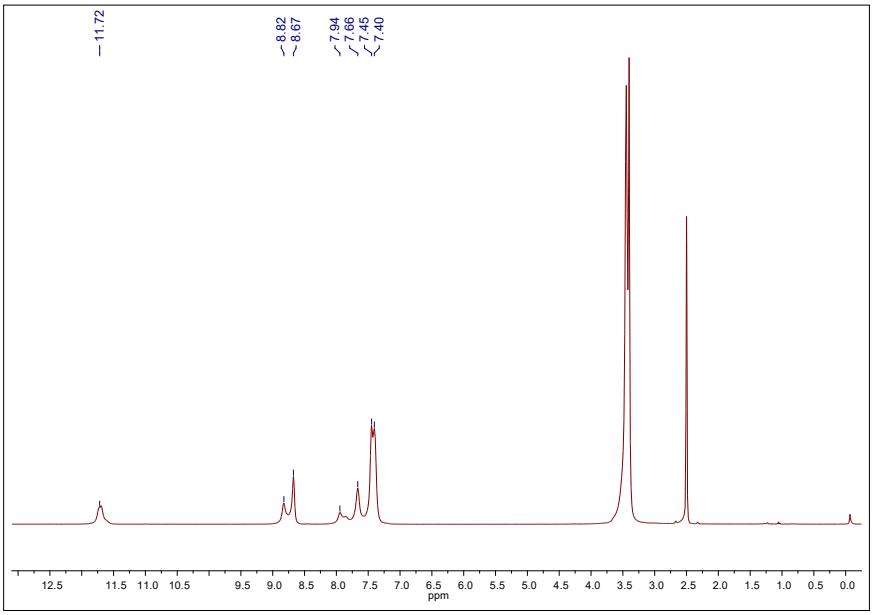

Fig. S7 ^{1}H NMR spectrum of H_2L in DMSO-d_6.

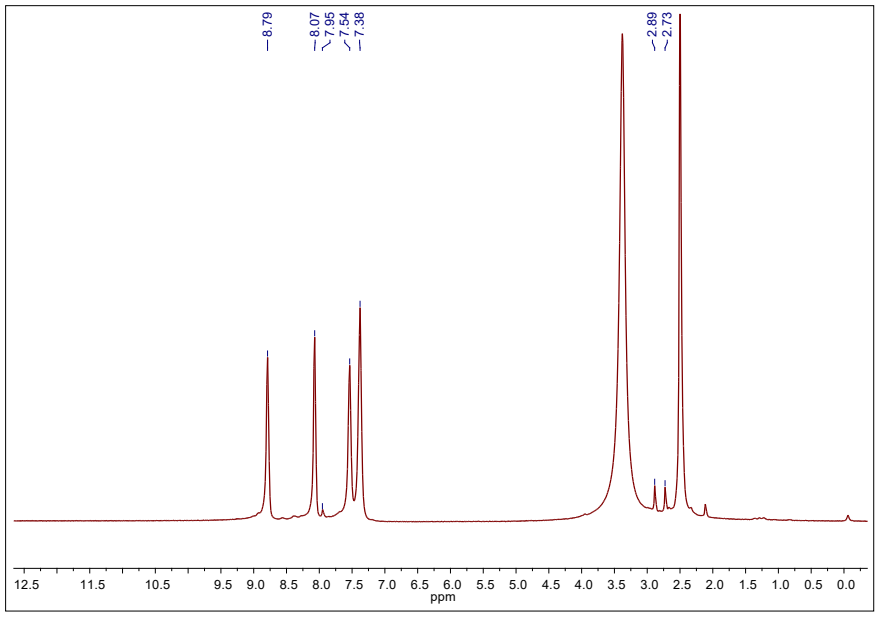

Fig. S8 ^{1}H NMR spectrum of UC in DMSO-$d_{6.}$

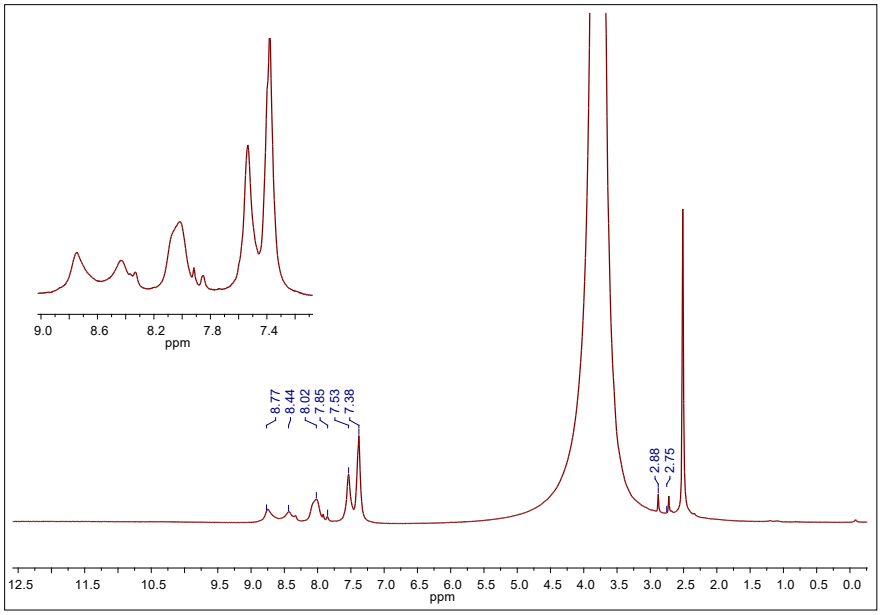

Fig. S9 ^{1}H NMR spectrum of UC in DMSO-d_6 after 1.5 hr of the PBS addition.

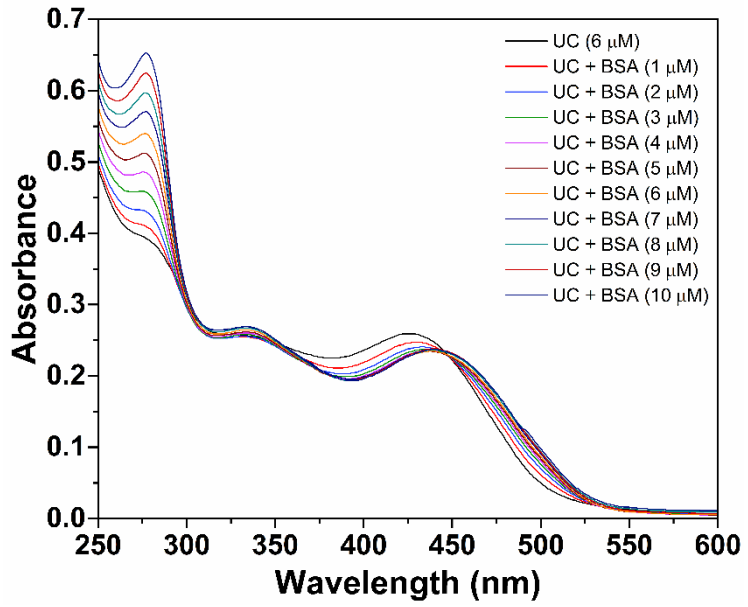

Fig. S10 UV-vis absorption spectra of UC in PBS with increasing concentration of BSA at 298 K.

(The binding constant, K_b was determined at a fixed wavelength of 427 nm using the formula: $[BSA]/(\varepsilon_a - \varepsilon_f) = [BSA]/(\varepsilon_b - \varepsilon_f) + 1/K_b(\varepsilon_b - \varepsilon_f)$. Where, ε_a represents the apparent absorption coefficient calculated from $A_{obs}/[UC]$, and ε_b and ε_c correspond to the extinction coefficients for UC while it was in the fully bound form and free form, respectively. The linear graph between $\{[BSA]/(\varepsilon_a - \varepsilon_f)\}$ *vs. [BSA]* provides the intercept value from which K_b was calculated).

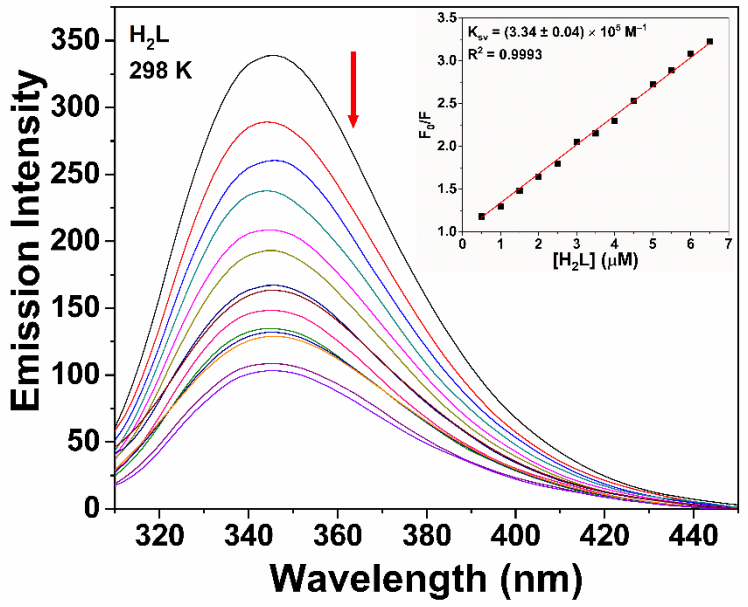

Fig. S11 The quenching effect of H_2L on BSA fluorescence at 298 K. Arrow shows the gradual decrease of emission intensity with increasing concentration of H_2L; Inset: Stern-Volmer plot for quenching of BSA fluorescence by H_2L.

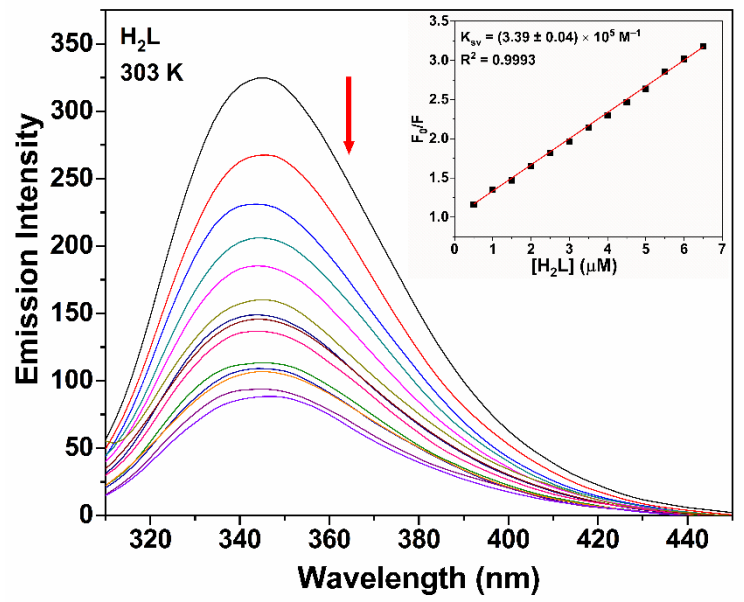

Fig. S12 The quenching effect of H_2L on BSA fluorescence at 303 K. Arrow shows the gradual decrease of emission intensity with increasing concentration of H_2L; Inset: Stern-Volmer plot for quenching of BSA fluorescence by H_2L.

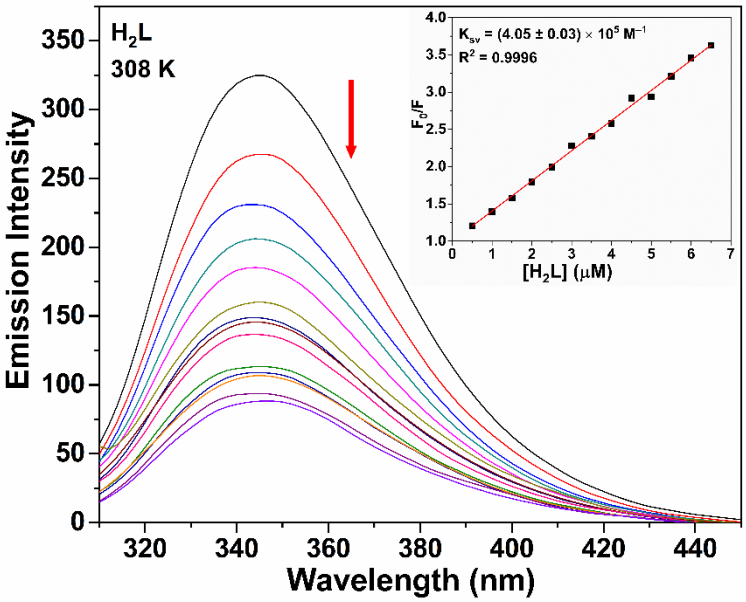

Fig. S13 The quenching effect of H_2L on BSA fluorescence at 308 K. Arrow shows the gradual decrease of emission intensity with increasing concentration of H_2L; Inset: Stern-Volmer plot for quenching of BSA fluorescence by H_2L.

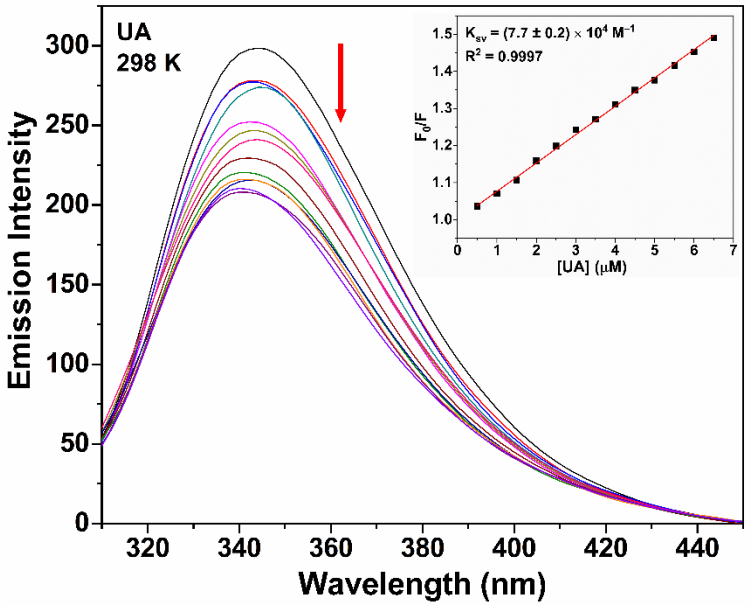

Fig. S14 The quenching effect of UA on BSA fluorescence at 298 K. Arrow shows the gradual decrease of emission intensity with increasing concentration of UA; Inset: Stern-Volmer plot for quenching of BSA fluorescence by UA.

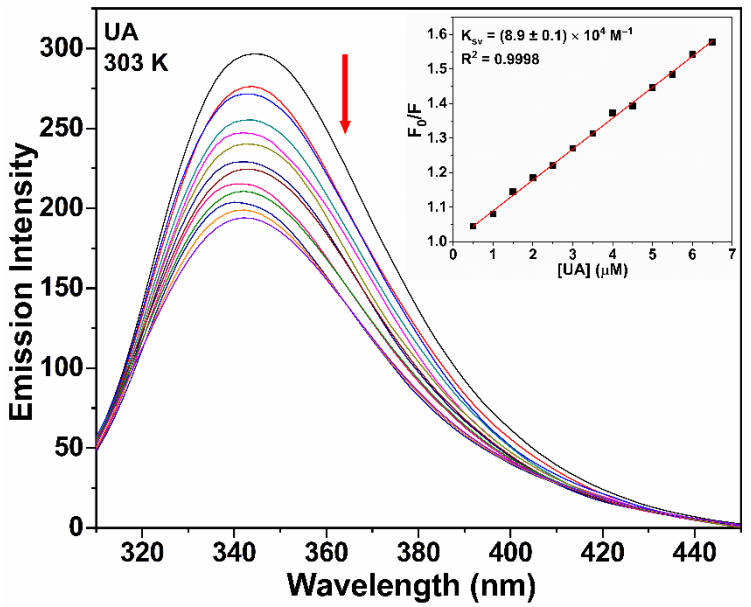

Fig. S15 The quenching effect of UA on BSA fluorescence at 303 K. Arrow shows the gradual decrease of emission intensity with increasing concentration of UA; Inset: Stern-Volmer plot for quenching of BSA fluorescence by UA.

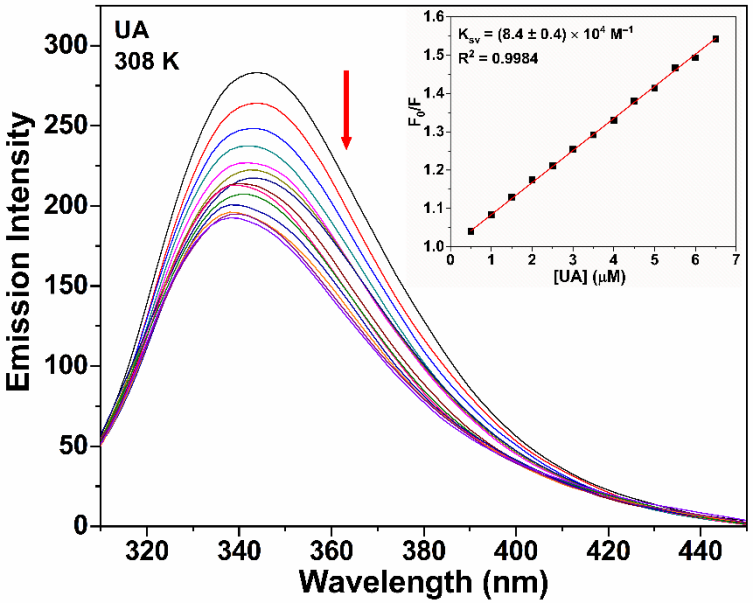

Fig. S16 The quenching effect of UA on BSA fluorescence at 308 K. Arrow shows the gradual decrease of emission intensity with increasing concentration of UA; Inset: Stern-Volmer plot for quenching of BSA fluorescence by UA.

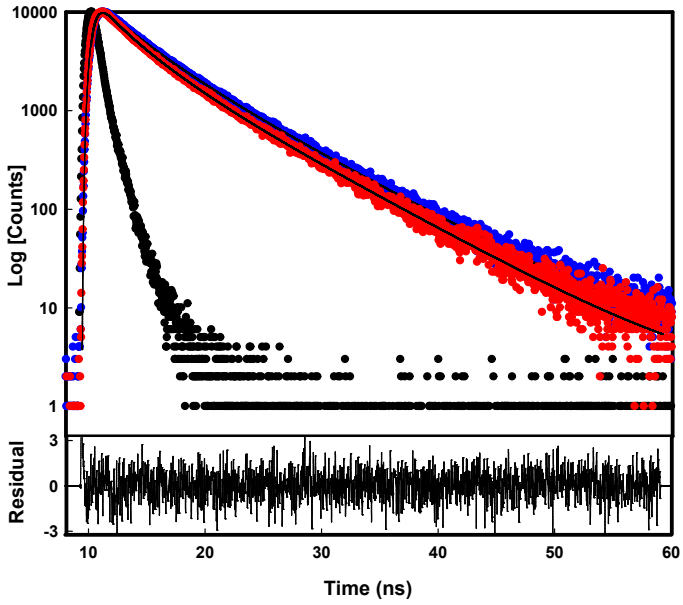

Fig. S17 Fluorescence lifetime decay profile of BSA in the absence and presence of UC at 298 K.

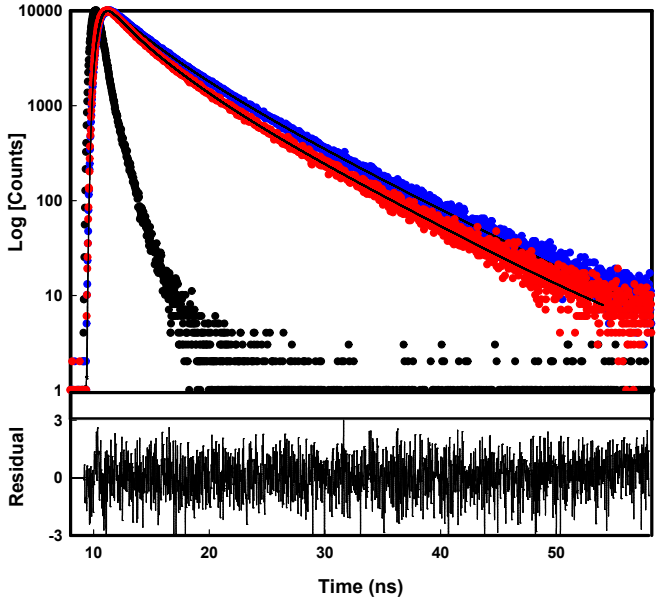

Fig. S18 Fluorescence lifetime decay profile of BSA in the absence and presence of UC at 303 K.

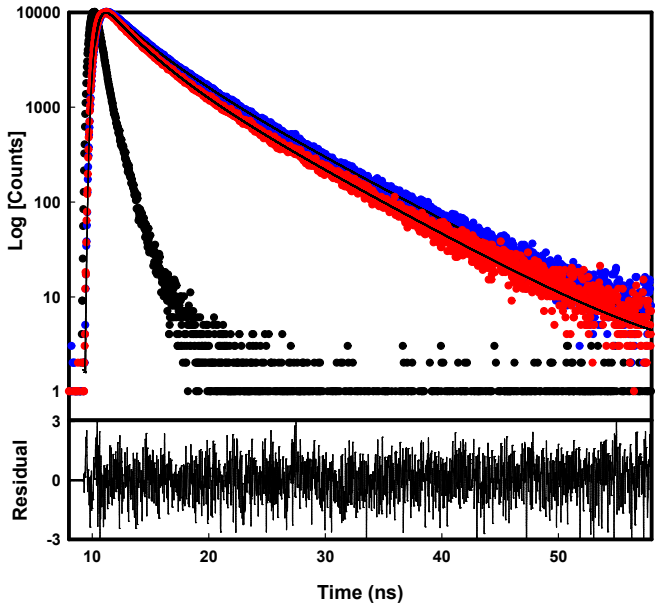

Fig. S19 Fluorescence lifetime decay profile of BSA in the absence and presence of UC at 308 K.

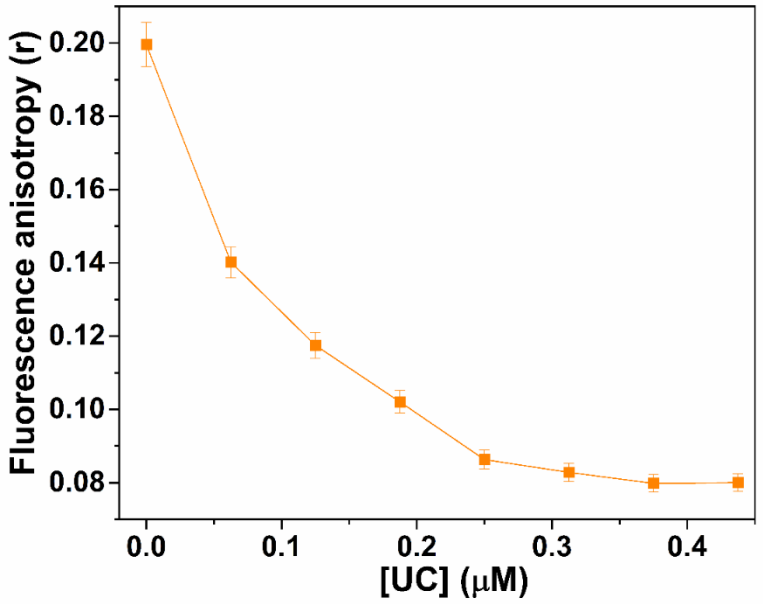

Fig. S20 The variation of fluorescence anisotropy of BSA with increasing concentration of UC. This experiment was carried out in PBS at 298 K and the concentration of BSA was kept constant at 1.0×10^{-6} M, and the emission was monitored at 343 nm by exciting at 295 nm.

Table S1 Selected bond lengths (Å) and bond angles (°) of UC.

Bond lengths		Bond angles			
U(1)–N(2)	2.5328	O(2)–U(1)–O(4)	88.916	O(1)–U(1)–O(3)	84.6615
U(1)–N(3)	2.5231	N(2)–U(1)–O(4)	88.3642	O(3)–U(1)–O(4)	89.5365
U(1)–O(1)	2.3654	N(2)–U(1)–O(2)	63.8766	O(3)–U(1)–O(5)	90.3992
U(1)–O(2)	2.302	N(3)–U(1)–O(4)	90.4756	O(1)–U(1)–O(4)	87.8806
U(1)–O(3)	2.3383	N(3)–U(1)–O(5)	88.3032	O(1)–U(1)–O(5)	93.4361
U(1)–O(4)	1.8166	N(3)–U(1)–N(2)	62.2522	O(4)–U(1)–O(5)	178.67
U(1)–O(5)	1.8137	N(3)–U(1)–O(3)	63.9188	O(2)–U(1)–O(5)	91.3783
		O(1)–U(1)–O(2)	85.2582	N(2)–U(1)–O(5)	90.6007

Table S2 Geometry of UC in XYZ format.

Atoms	X	Y	Z
C	4.75365	3.72281	−0.36806
C	3.71379	2.79630	−0.58897
C	2.58661	2.76096	0.27507
C	2.53565	3.65820	1.37516
C	3.58815	4.56839	1.60836
C	4.69768	4.60987	0.73327
H	5.61062	3.74836	−1.05013
H	3.76993	2.10018	−1.43046
H	1.67728	3.63588	2.05478
H	3.53822	5.24647	2.46715
H	5.51075	5.32353	0.90756
C	1.46857	1.79954	0.04882
C	0.06421	2.24389	0.03731
C	−0.29324	3.69158	−0.01139
C	0.29568	4.53400	−0.99134
C	−1.22422	4.24878	0.90558
C	−0.04271	5.90228	−1.05718
H	1.00976	4.11510	−1.70811
C	−1.54304	5.62134	0.85382
H	−1.69123	3.60507	1.65647
C	−0.95782	6.45280	−0.13071
H	0.41186	6.53674	−1.82565
H	−2.25204	6.04141	1.57578
H	−1.21313	7.51753	−0.17504
N	−0.85063	1.25715	0.02103
N	1.64844	0.47529	−0.10541
N	2.95914	−0.00573	−0.05436
N	−2.19422	1.63594	−0.05157
C	2.96918	−1.35143	−0.19794
C	−2.99889	0.55036	−0.07048
C	4.28143	−2.04359	−0.17363
C	4.35052	−3.44223	−0.39500
C	5.49068	−1.34013	0.06866
C	5.61246	−4.07374	−0.36806
H	3.43309	−4.00651	−0.58460
C	6.70278	−2.06117	0.07810
H	5.46607	−0.26213	0.24882
H	5.70250	−5.15269	−0.53768
H	7.65468	−1.55164	0.26466
C	−4.46238	0.79053	−0.16643
C	−5.36498	−0.29799	−0.26580
C	−5.00001	2.10504	−0.16578

C	−6.74884	−0.03397	−0.35179
H	−4.98220	−1.32174	−0.28778
C	−6.39802	2.26777	−0.25408
H	−4.32784	2.96478	−0.10390
H	−7.47184	−0.85380	−0.43297
H	−6.84479	3.26816	−0.25569
O	1.85915	−2.06550	−0.36641
O	−2.54075	−0.69931	−0.00472
U	−0.26035	−1.18817	−0.17373
O	−0.39330	−1.02847	−1.97553
O	−0.13611	−1.30786	1.63466
O	−1.05457	−3.41619	−0.19155
N	−7.28190	1.22514	−0.34492
N	6.78671	−3.41154	−0.13579
C	−1.43246	−4.57988	0.16636
H	−0.75564	−5.44470	0.04817
N	−2.64483	−4.86681	0.69964
C	−3.65666	−3.81428	0.93518
H	−4.57952	-4.05667	0.37690
H	−3.89428	−3.75958	2.01283
H	−3.27054	−2.83833	0.60321
C	−3.00327	−6.24642	1.07955
H	−3.22460	−6.29866	2.16065
H	−3.89563	−6.57714	0.51822
H	−2.17021	−6.93283	0.85608

Table S3 Binding parameters of BSA-H_2L and BSA-UA systems at three different temperatures.

H_2L/UA	T(K)	K_{sv} ($L.mol^{-1}$)	R^2	k_q ($L.mol^{-1}.s^{-1}$)
H_2L	298 K	$(3.34 \pm 0.04) \times 10^5$	0.9993	$(5.51 \pm 0.06) \times 10^{13}$
	303 K	$(3.39 \pm 0.04) \times 10^5$	0.9993	$(5.59 \pm 0.06) \times 10^{13}$
	308 K	$(4.05 \pm 0.03) \times 10^5$	0.9996	$(6.68 \pm 0.04) \times 10^{13}$
UA	298 K	$(7.7 \pm 0.2) \times 10^4$	0.9997	$(1.27 \pm 0.03) \times 10^{13}$
	303 K	$(8.9 \pm 0.1) \times 10^4$	0.9998	$(1.47 \pm 0.02) \times 10^{13}$
	308 K	$(8.4 \pm 0.4) \times 10^4$	0.9984	$(1.39 \pm 0.06) \times 10^{13}$

Table S4 Fluorescence lifetime decay of BSA (1.0×10^{-6} M) in the absence and presence of UC in PBS at three different temperatures.

T (K)	[UC] (μM)	α_1	τ_1 (ns)	α_2	τ_2 (ns)	α_3	τ_3 (ns)	$<\tau>$ (ns)	χ^2
298	0	32.92	3.17	2.91	6.65	64.17	6.81	6.127015	1.01
	1.0	36.8	3.02	58.39	6.73	4.81	1.15	5.860392	1.28
303	0	37.19	3.53	54.01	7.04	8.81	1	6.052134	1.07
	1.0	40.28	3.07	49.13	6.7	10.59	7.69	6.010717	1.06
308	0	36.41	3.05	6.15	7.61	57.44	6.65	5.992657	1.03
	1.0	37.59	2.75	11.46	7.34	50.94	6.42	5.833069	1.04

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