Supplementary Materials for:

Photoacids as a new fluorescence tool for tracking structural transitions of proteins: Following the concentration-induced transition of bovine serum albumin

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Table S1. k_{PT} values as calculated by Eq. (2) for all the steady-state curves. The BSA concentrations are in % w/v and the k_{PT} values are in $\times 10^9$ s^{-1}.

	HPTS	0.001	0.005	0.01	0.03	0.05	0.075	0.1	0.3	0.5
pH7 170µM	17.5	17.7	17.6	16.8	16.7	15.5	15.2	12.0	9.53	6.95
pH7 20µM	13.0	10.9	9.53	7.46	5.91	4.79	4.18	3.47	2.69	2.37
pH2 170µM	1.69	1.41	1.36	1.03	0.67	0.54	0.41	0.33	0.21	0.17
pH2 20µM	1.63	1.30	0.88	0.49	0.25	0.18	0.15	0.14	0.13	0.12

	0.75	1	1.5	2	2.5	3	4	5	6	7	8
pH7 170µM	4.62	3.95	3.26	2.89	2.79	2.64	2.55	2.44	2.40	2.40	2.43
pH7 20µM	2.20	2.07	1.92	1.85	1.78	1.82	1.80	1.75	1.74	1.68	1.66
pH2 170µM	0.18	0.21	0.28	0.43	0.53	0.65	0.83	1.01	1.21	1.34	1.50
pH2 20µM	0.12	0.14	0.17	0.24	0.32	0.41	0.53	0.69	0.76	0.89	0.96

Table S2. K2D3 analysis of the CD spectrum showing the calculated percentage of α-helix and β-sheet at the different BSA concentrations and at the different pH values.

BSA weight conc. (%w/v)	pH7		pH2	
	α-helix (%)	β-sheet (%)	α-helix (%)	β-sheet (%)
0.01	68.2	8.6	57.6	9.0
0.03	68.2	8.6	59.7	8.8
0.05	68.2	8.7	58.3	8.9
0.075	68.1	8.7	60.7	8.5
0.1	68.1	8.6	61.1	8.1
0.3	67.6	9.0	60.9	8.9
0.5	67.8	9.0	61.0	8.1
0.75	67.8	9.0	60.4	8.2
1	68.0	8.9	54.9	8.0

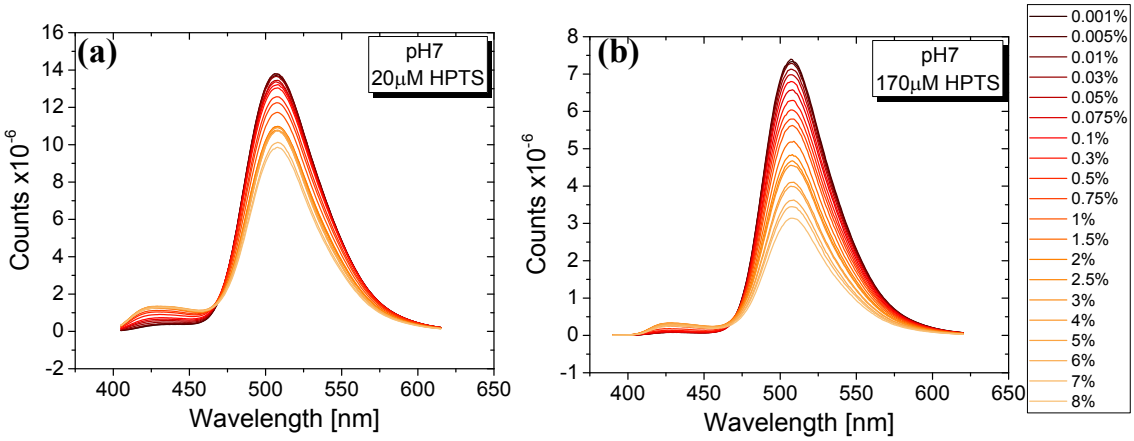

Figure S1. Un-normalized steady-state emission of (a) 20 μM and (b) 170 μM at pH7 in different BSA weight concentration.

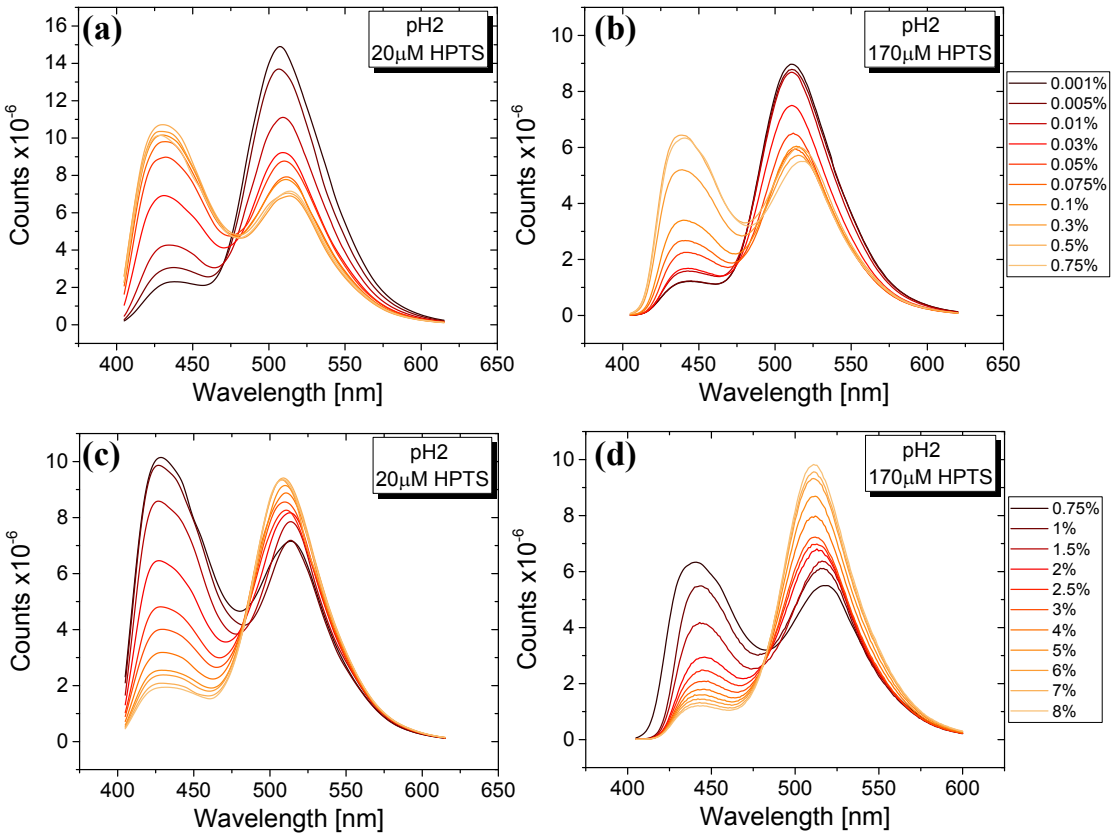

Figure S2. Un-normalized steady-state emission of (a and c) 20µM and (b and d) 170µM at pH2 in different BSA weight concentration at the range of (a and b) 0.001-0.75% and (c and d) 0.75-8%.

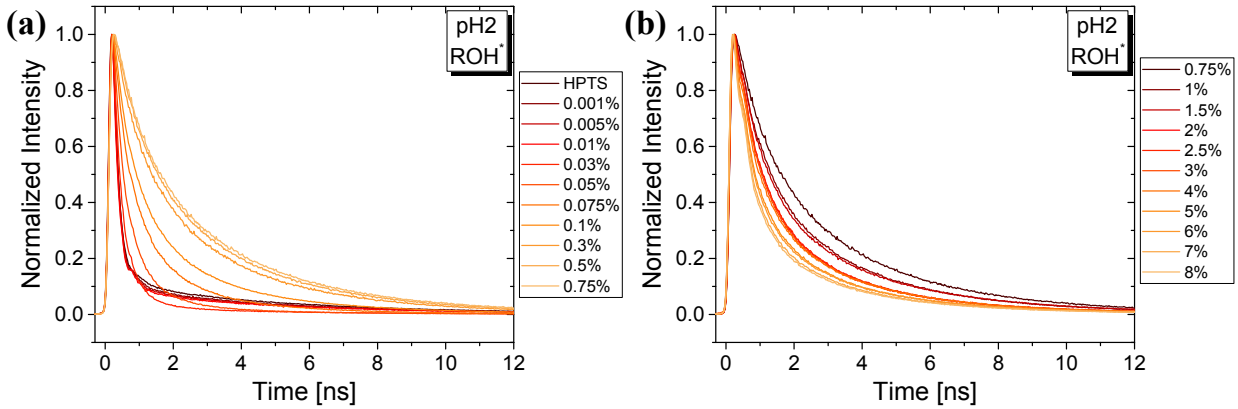

Figure S3. Time-resolved emission of HPTS at pH2 at the emission wavelengths of ROH^* on a linear scale in BSA fractions of (a) ≤0.75% and (c) ≥0.75%.

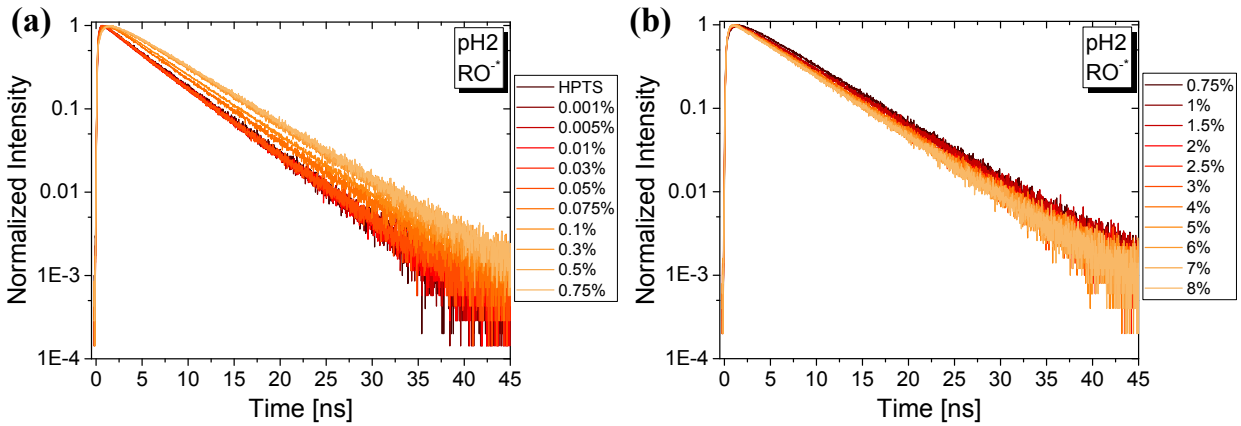

Figure S4. Time-resolved emission of HPTS at pH2 at the emission wavelengths of RO^{-*} on a semi-log scale in BSA fractions of (a) ≤0.75% and (c) ≥0.75%.

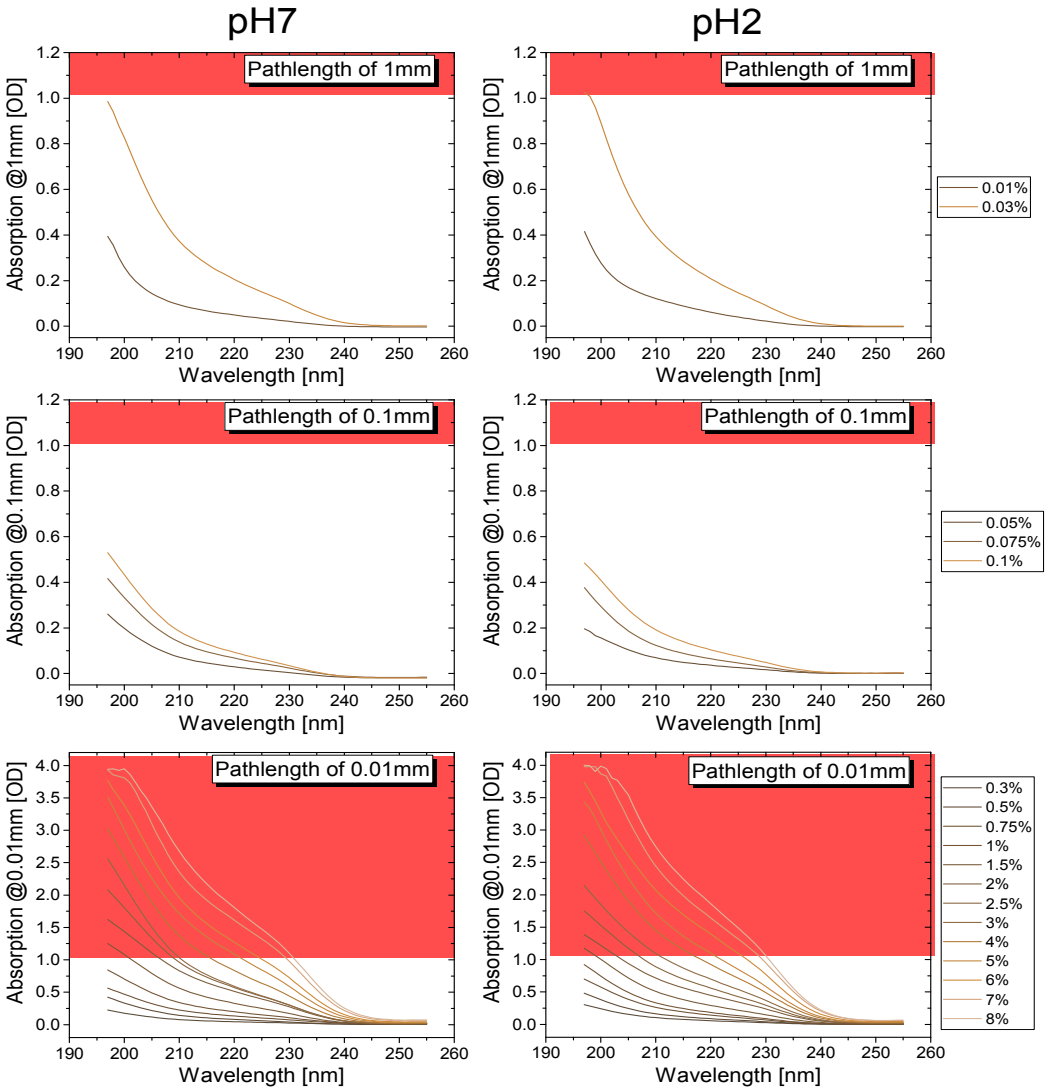

Figure S5. The corresponding absorption spectrum of the CD spectrum (Figure 13 in the main text). The red areas indicate the absorption values (>1OD) that result in an unreliable CD spectrum.