Tyrosine fluorescence probing of the surfactant-induced conformational changes of albumin

Nadezda G. Zhdanova[a], Evgeny A. Shirshin[a,*], Eugene G. Maksimov[b], Ivan M. Panchishin[a], Alexander M. Saletsky[a] and Victor V. Fadeev[a].

[a] Department of Physics, M.V. Lomonosov Moscow State University, Moscow 119991, Russia.
[b] Department of Biology, M.V. Lomonosov Moscow State University, Moscow 119991, Russia.
[*] Corresponding author: shirshin@lid.phys.msu.ru.

Electronic Supplementary Information

1. Comparison of Raman emission from water and fluorescence of BSA

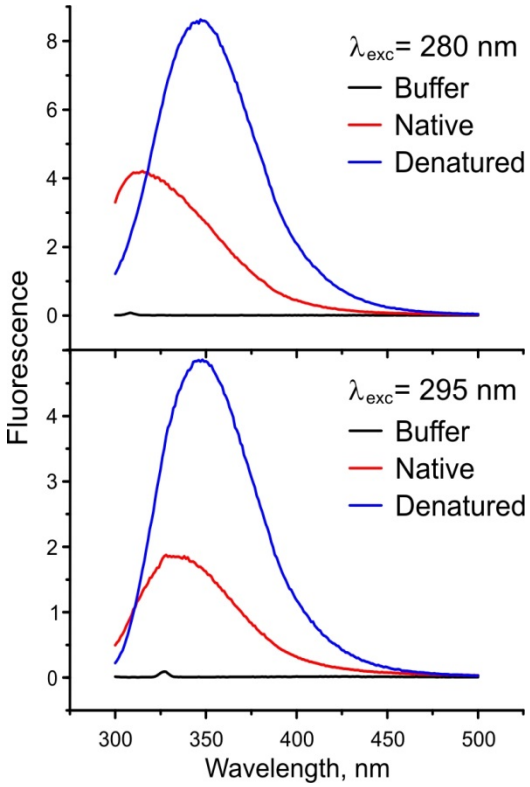

Fig. S1. Comparison between Raman emission from water and fluorescence of BSA

2. Fluorescence decay parameters for BSA in presence and absence of [SDS]

Fluorescence decay curves were obtained using two registration wavelengths (318 and 355 nm for Tyr+Trp and Trp respectively). The former one was fitted by a sum of three exponential decay functions, while the latter was fitted by a biexponential decay.

The shortest lifetime obtained at 318 nm registration wavelength was attributed to Tyr as it has non-monotonous dependence on SDS concentration.

Lifetimes values and its relative amplitudes are presented in the Tables S1 and S2. Representative emission decay curves for two registration wavelengths (318 and 355 nm) are presented in Figs. S2 and S3. Statistical data (χ^2) for fitting of decays obtained at two registration wavelengths are listed

in Table S3.

Table S1. Lifetimes (t_i. ps) and its relative amplitudes (a_i) for Tyr (1) and Trp (2. 3) obtained at registration wavelength of 318 nm.

[SDS], mM	a_1, %	t_1, ps	a_2, %	t_2,ps	a_3, %	t_3, ps
0.00	68.8	1484	25.3	5215.5	5.8	8198.8
10.91	67	1799	22.5	2812.4	10.5	4381.5
9.11	65.6	1848	22.1	2521.1	12.3	4341.6
7.59	61.2	1904	24.2	2231.5	14.6	4169.4
6.33	69.2	1762	18	2741.8	12.8	4130.1
5.27	66.4	1767	20.2	2609.6	13.4	4122.9
4.39	60.8	1842	26.3	2341.4	12.9	4320.2
3.66	68.5	1817	18.5	2740.9	13	4283.5
3.05	68.9	1810	15.5	2607.1	15.6	4212.8
2.54	71.8	1809	15.6	2929.7	12.6	4425.1
2.12	73.8	1836	16.6	3363.7	9.6	4796.7
1.77	73.2	1940	20.6	3992.6	6.3	5622
1.47	64	1977	30.2	4218.4	5.8	5987.9
1.23	63.6	2056	31.2	4693.2	5.2	5341.3
1.02	60.5	2048	33.9	4692.4	5.5	5264.6
0.85	60.6	2128	34	4684.4	5.4	5514.1
0.71	61.8	2150	32.8	4707.5	5.4	5720.2
0.59	60.2	2087	34.2	4743.6	5.6	5253.3
0.49	59.3	2028	35.2	4624.2	5.5	5504
0.40	60.6	2106	33.6	4730.4	5.8	5238.7
0.34	59.8	2043	34.9	4566.9	5.4	5864.2
0.29	63.1	2106	31.4	4773.6	5.6	5492.6
0.24	65.2	2157	29.3	4836.3	5.5	5700.1
0.20	63.5	2099	31.1	4710.2	5.4	5760.6
0.17	65.2	2111	29.1	4768.6	5.7	5740.9
0.14	65.5	2087	28.3	4607.8	6.3	6304.8
0.12	62.8	2054	30.9	4385.9	6.2	6552.1
0.096	63.9	1998	29.7	4425.6	6.4	6501.3
0.080	64.4	1930	30.3	4436.7	5.4	6836
0.066	71.2	2029	22.9	4834.6	5.9	6600.2
0.055	67.7	1803	26.2	4399.4	6.1	7221.9
0.046	69.7	1783	25.2	4683.7	5	7539.9
0.038	65.5	1592	28.1	4209.9	6.4	7801.3
0.032	64.9	1556	28.4	4273.7	6.7	7792
0.027	66.3	1546	27.4	4403.2	6.3	8067.1
0.022	70	1633	24.5	4983.5	5.5	7828.6
0.019	70.1	1579	23.9	4998.5	6	7770.9
0.015	70.2	1580	24.3	5180.1	5.4	7779.1
0.013	69.4	1562	24.9	5028.2	5.7	8098.7
0.011	68.3	1501	26.4	4952.3	5.3	8444.3
0.0089	68.2	1502	25.9	4977.8	5.9	8088.2
0.0074	68.5	1504	25.9	5140.2	5.6	7928.5
0.0062	67.1	1453	27.1	4883.7	5.8	8315.4
0.0052	66.9	1456	26.8	4772.6	6.3	8446.4

Table S2. Lifetimes (τ_i) and its relative amplitudes (a_i) for Trp obtained at 355 nm registration wavelength.

[SDS], mM	a1, %	t1, ps	a2, %	t2, ps
0.00	83.5	5692	16.5	8845.8
10.91	79.6	2206	20.4	4576.4
9.11	82.7	2265	17.3	4694.3
7.59	81.1	2192	18.9	4568.2
6.33	80.8	2182	19.2	4524
5.27	79.9	2155	20.1	4482.4
4.39	79.5	2209	20.5	4511.6
3.66	78.2	2301	21.8	4660.6
3.05	76.7	2332	23.3	4714.5
2.54	75.8	2380	24.2	4784
2.12	72.9	2397	27.1	4886.1
1.77	67.7	2620	32.3	5153.3
1.47	63	2968	37	5367.5
1.23	67.5	3385	32.5	5660.2
1.02	68.7	3509	31.3	5749
0.85	69.2	3552	30.8	5790.6
0.71	69.2	3513	30.8	5850.6
0.59	66.1	3449	33.9	5735
0.49	67.5	3471	32.5	5829.6
0.40	72.1	3527	27.9	6067.9
0.34	70.8	3484	29.2	6039.6
0.29	66.5	3353	33.5	5911.8
0.24	66.5	3347	33.5	5972.4
0.20	66.2	3354	33.8	6014.6
0.17	67.2	3329	32.8	6172.7
0.14	68.8	3360	31.2	6372.2
0.12	67.7	3315	32.3	6492.6
0.096	64.5	3258	35.5	6550.2
0.080	64	3296	36	6803.7
0.066	61.3	3320	38.7	6928.8
0.055	57.3	3358	42.7	6972.6
0.046	55.5	3517	44.5	7046.6
0.038	51	3673	49	6981
0.032	53.6	4006	46.4	7163.8
0.027	53.6	4200	46.4	7165.3
0.022	69.1	4782	30.9	7860.8
0.019	71.4	4958	28.6	7972.1
0.015	71.7	5031	28.3	7987.2
0.013	72.4	5126	27.6	8017
0.011	75.4	5226	24.6	8204
0.0089	78.6	5380	21.4	8347.2
0.0074	75.3	5316	24.7	8143.8
0.0062	80	5453	20	8435.9
0.0052	82.5	5539	17.5	8601.7

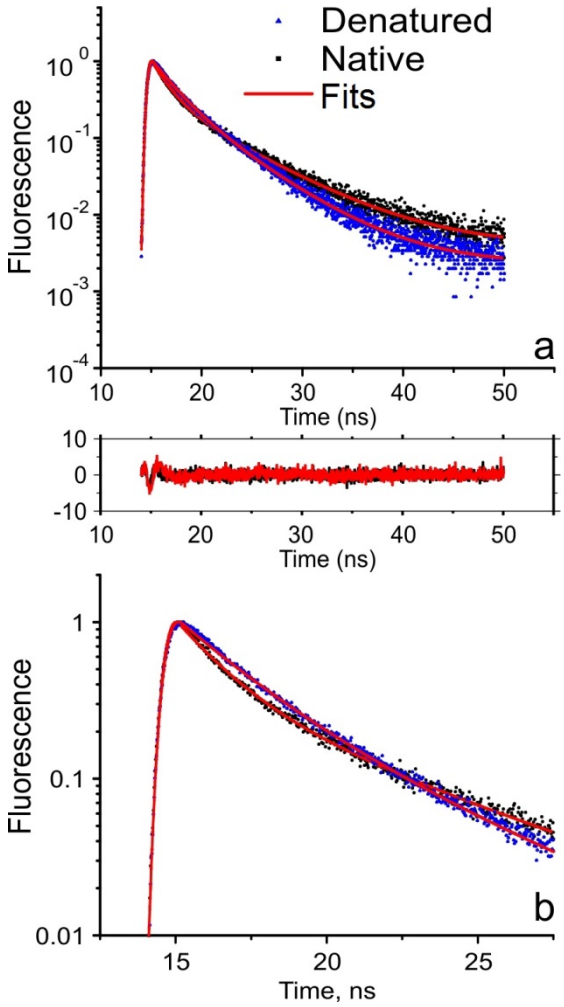

Fig. S2. a) Fluorescence decay curves for native ([SDS] = 0) and denatured ([SDS] = 0.16 mM) BSA measured at 318 nm, its fit by a sum of three exponential decays (red line) and corresponding residuals. b) Enlarged initial stage of the fluorescence decay curves for native ([SDS] = 0) and denatured ([SDS] = 0.16 mM) BSA, its fit by a sum of three exponential decays. Registration wavelength is 318 nm.

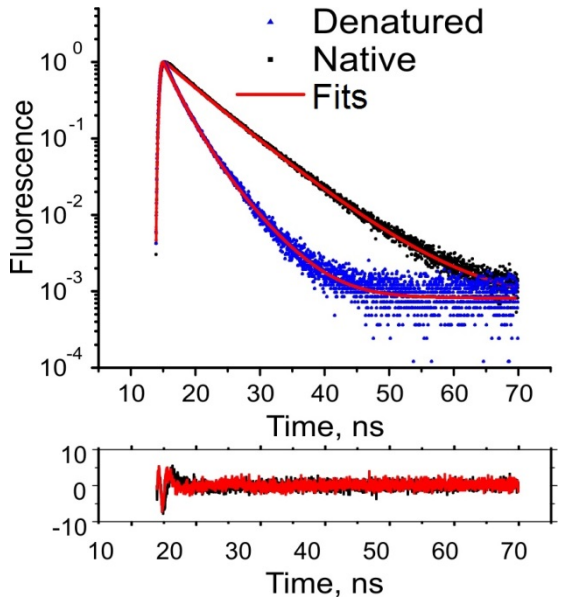

Fig. S3. Fluorescence decay curves for native ([SDS] = 0) and denatured ([SDS] = 0.16 mM.

lifetime for Tyr is maximum) BSA, its fit with a biexponential decay and corresponding residuals. Registration wavelength is 355 nm.

Table S3. Statistical data (χ^2) for fitting of fluorescence decays obtained at two registration wavelengths.

[SDS], mM	3 exp 318 nm	2 exp 355 nm
0.00	1.15	1.63
10.91	1.51	1.56
9.11	1.47	1.70
7.59	1.47	1.60
6.33	1.37	1.52
5.27	1.45	1.51
4.39	1.49	1.53
3.66	1.55	1.49
3.05	1.43	1.51
2.54	1.48	1.57
2.12	1.54	1.51
1.77	1.40	1.56
1.47	1.37	1.57
1.23	1.26	1.48
1.02	1.29	1.49
0.85	1.28	1.51
0.71	1.26	1.52
0.59	1.29	1.52
0.49	1.21	1.53
0.40	1.23	1.47
0.34	1.20	1.59
0.29	1.20	1.55
0.24	1.23	1.54
0.20	1.24	1.56
0.17	1.26	1.49
0.14	1.29	1.54
0.12	1.22	1.62
0.096	1.27	1.64
0.080	1.22	1.47
0.066	1.24	1.43
0.055	1.22	1.41
0.046	1.19	1.46
0.038	1.14	1.48
0.032	1.19	1.43
0.027	1.18	1.54
0.022	1.18	1.48
0.019	1.18	1.60
0.015	1.15	1.45
0.013	1.19	1.57
0.011	1.11	1.52
0.0089	1.13	1.56
0.0074	1.22	1.59
0.0062	1.13	1.65
0.0052	1.10	1.61

3. **Determnation of critical micelle concentration (CMC) for SDS in Tris-buffer by means of pyrene (Py) fluorescence**

We used pyrene (Py) as a fluorescent probe to determine CMC. CMC determination implies the measurement of the ratio of the intensities of the first (373 nm) and the third (384 nm) vibronic peaks in pyrene's fluorescence spectrum (Kalyanasundaram & Thomas 1977) – I_1/I_3 (Fig. S4).

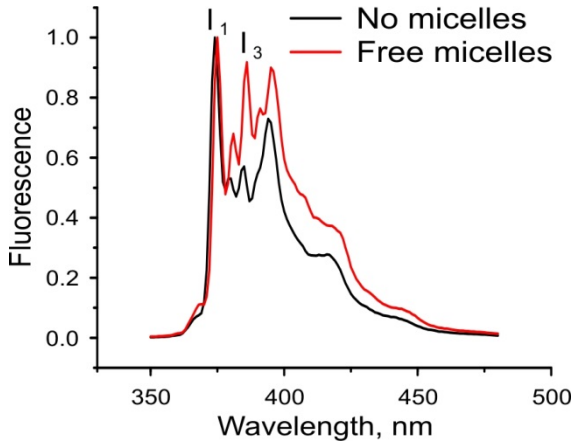

Fig. S4. Py fluorescence spectra in solution with (red) and without (black) micelles in solution. Excitation wavelength is 334 nm. Py concentration is 0.5 μM.

Fig. S5 displays the I_1/I_3 ratio as a function of SDS concentration for two solvents: water and Tris-buffer. It can be seen from this data that in water CMC of SDS determined by Py fluorescence is 8 mM that is in accordance with the literature (Otzen 2011; Kalyanasundaram & Thomas 1977). Also it should be noted that in buffer solution used in our investigations CMC significantly decreases and is only 0.7 mM, that is also in accordance with the literature data (Otzen 2011; Kalyanasundaram & Thomas 1977).

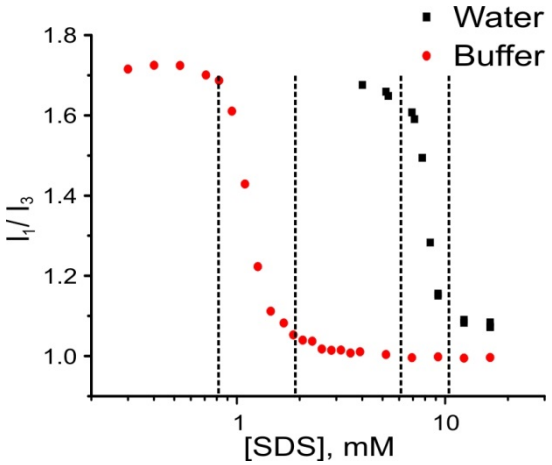

Fig. S5. The I_1/I_3 ration as a function of SDS concentration in water (black squares) and in Tris-buffer (red circles), excitation wavelength is 334 nm, λ_1 = 373 nm and λ_2 = 384 nm