Quaternary Structure Analysis of a Hemoglobin Core in Hemoglobin−Albumin Cluster

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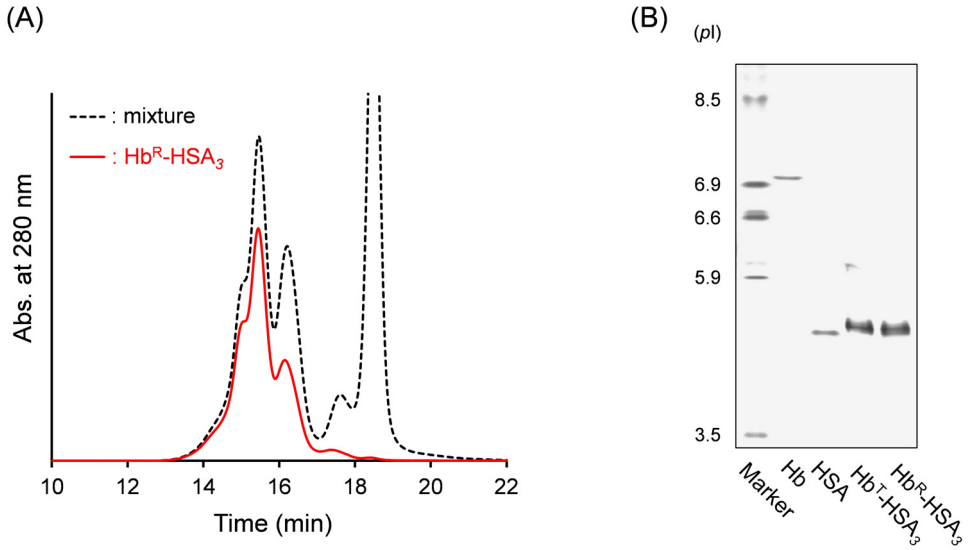

Figure S1. (A) SEC chromatograms of Hb^R–HSA_3 cluster (solid line) and reaction mixture (dotted line). (B) IEF of Hb^R–HSA_3 and Hb^T–HSA_3 clusters.

Table S1. UV-vis Absorption Spectral Data of Hb and $Hb^{R(or\ T)}$–HSA_3 cluster in PBS Solution (pH 7.4, 25 °C)

hemeprotein	λ_{max} (nm)			
	deoxy	oxy	carbonyl	nitrosyl
Hb	430	414	420	418
	555	541	538	544
		577	569	574
Hb^R–HSA_3	430	414	420	418
	556	541	538	543
		577	569	572
Hb^T–HSA_3	430	414	419	417
	555	542	538	544
		577	568	572

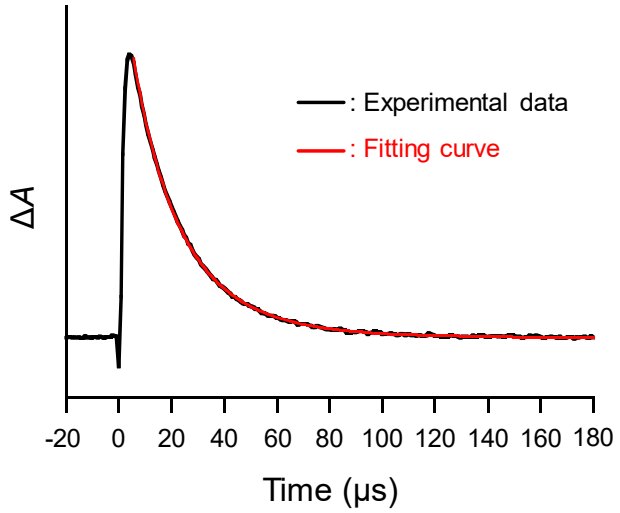

Figure S2. Absorption decay of O_2 rebinding to Hb^R–HSA_3 cluster in PBS solution (pH 7.4) after the laser flash photolysis at 25 °C (λ = 436 nm). The kinetics was composed of two phases. A relaxation curve was fitted double-exponentials.

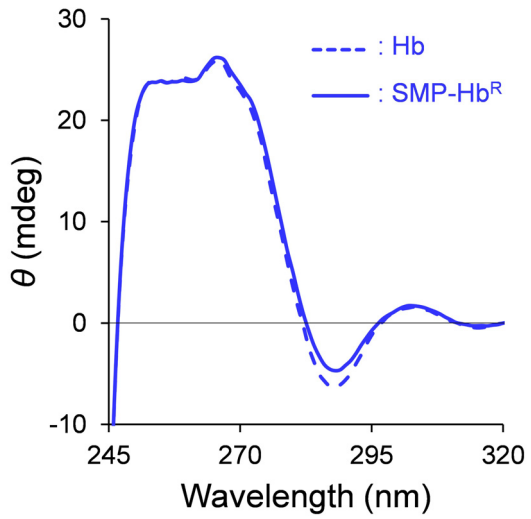

Figure S3. CD spectra of deoxy Hb (dotted line) and SMP-Hb^T (solid line) in PBS solution (pH 7.4) at 25 °C (Protein] = 20 μM).

Table S2. X-ray Crystallography Data Collection and Refinement Statistics of Carbonyl Hb^R and SNP-Hb^R

	Carbonyl Hb^R	Carbonyl SNP-Hb^R
Wavelength (Å)	1.0000	0.9000
Resolution range (Å)	1.34 – 48.83 (1.34 – 1.36)	1.460 – 45.50 (1.460 – 1.490)
Space group	P 21 21 21	P 21 21 21
Cell dimensions	*a* = 63.56Å, *b* = 76.28Å, *c* = 109.79Å, α = 90.00°, β = 90.00°, γ = 90.00°	*a* = 65.12Å, *b* = 78.13Å, *c* = 109.54Å, α = 90.00°, β = 90.00°, γ = 90.00°
Unique reflections	120044 (5862)	96527 (4759)
Multiplicity	14.5 (14.4)	8.7 (7.4)
Completeness (%)	99.8 (99.6)	99.4 (99.7)
Mean I/sigma (I)	20.3 (2.0)	7.1(2.0)
R-merge	0.076 (1.517)	0.076 (0.933)
Refinement		
Resolution range (Å)	1.34 – 48.83 (1.340 – 1.375)	1.46 – 45.50 (1.46 – 1.49)
No. reflections	117962 (8592)	92155 (6074)
R-work	0.1374 (0.2300)	0.1453 (0.2040)
R-free	0.1753 (0.2800)	0.1996 (0.2520)
No. non-hydrogen atoms	5230	5218
Macromolecules	4327	4357
RMS (bonds)	0.0129	0.0113
RMS (angles)	1.42	1.22
Ramachandran favored (%)	98.38	98.93
Ramachandran outliers (%)	0.00	0.00
Clashscore	2.90	3.54
Average B-factor	22.0	30.0

Statistics for the highest-resolution shell are shown in parentheses.