Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Physiological concentrations of albumin favor drug binding

D. Tatlidil,[a] M. Ucuncu,[b] and Y. Akdogan[a]

[a]Materials Science and Engineering Department, İzmir Institute of Technology, 35430 Urla, İzmir, Turkey
[b]Department of Chemistry, İzmir Institute of Technology, 35430 Urla, İzmir, Turkey

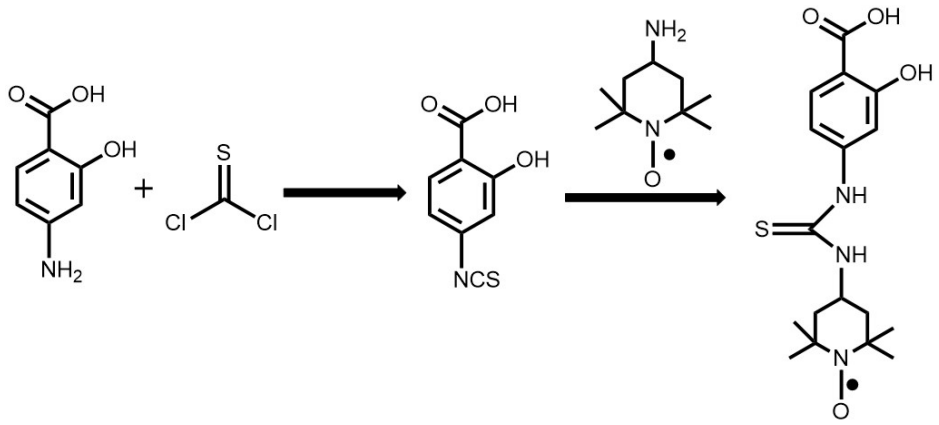

Fig. S1. Synthetic route to spin labeled salicylic acid (SLSA) from 4-amino salicylic acid.

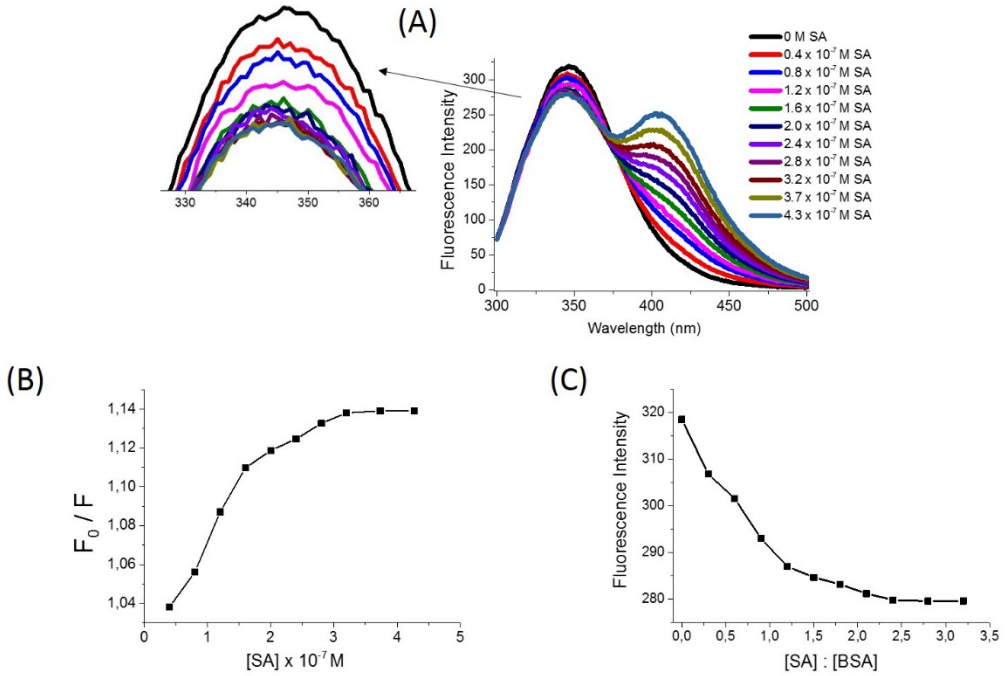

Fig. S2. (A) Fluorescence emission spectra of BSA (1.5 x 10^{-7} M) in the presence of SA with different concentrations (0-4.3 x 10^{-7} M) at 303 K. (B) Stern-Volmer plot of the SA-BSA complexes. F_0 and F are the fluorescence intensities of the BSA before and after the addition of the SA (quencher), respectively. (C) Fluorescence quenching ceased above the ratio of ~2:1 for SA-BSA.

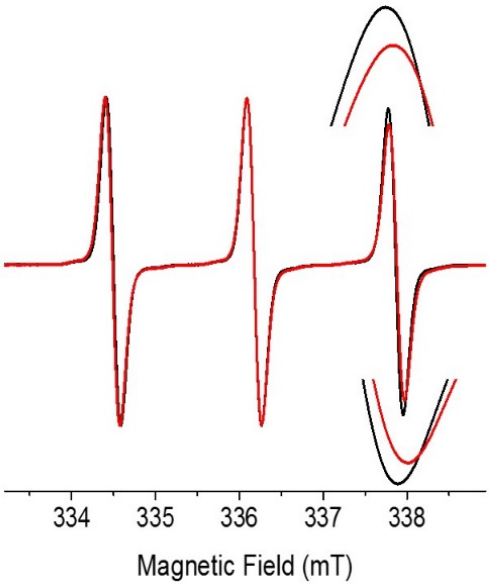

Fig. S3. EPR spectra of SLSA (red) and Tempo-4-amino (black) in 0.1 M phosphate buffer solutions containing 1% (v/v) DMSO.

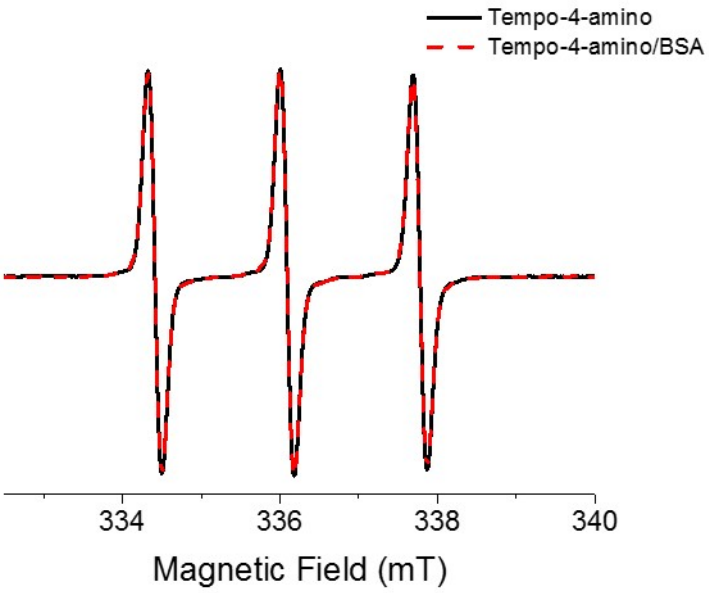

Fig. S4. EPR spectra of 0.5 mM Tempo-4-amino (black) and 0.5 mM Tempo-4-amino/BSA complex (1:1) (red dashed line) in 0.1 M phosphate buffer solutions.

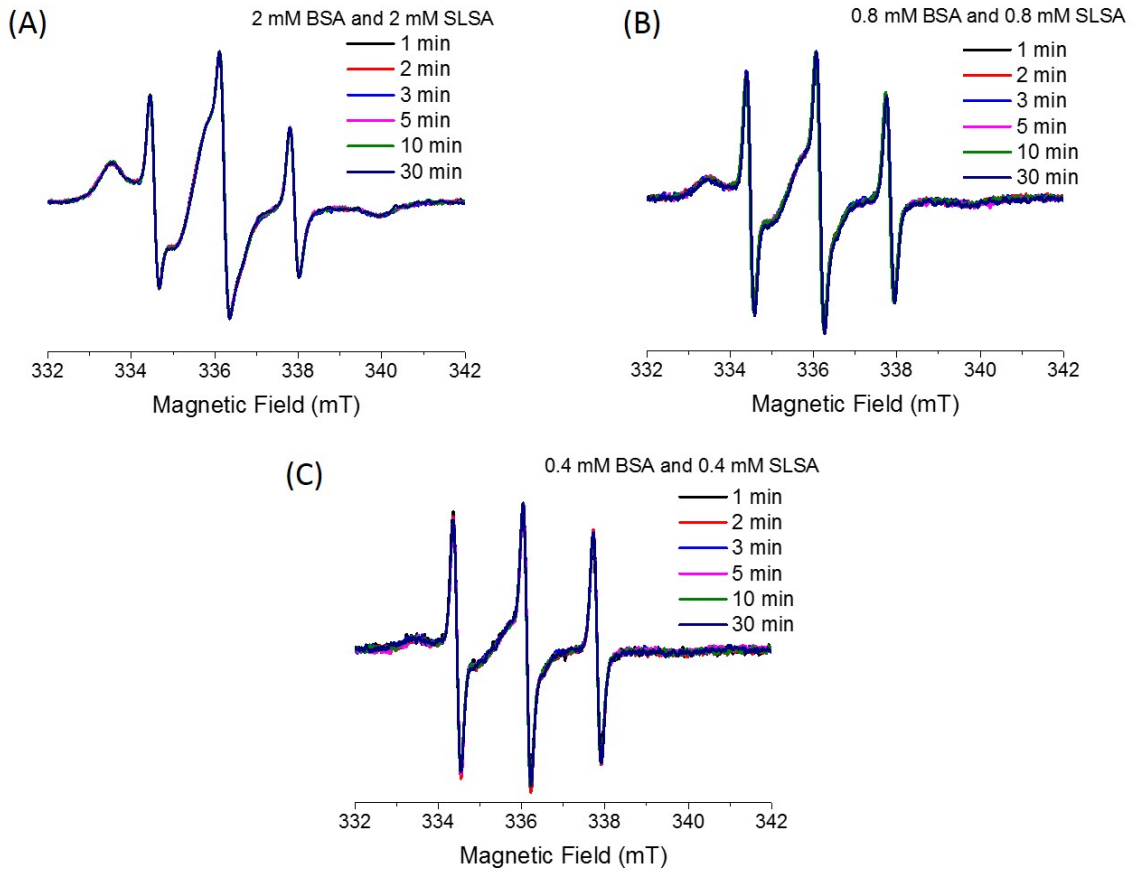

Fig. S5. EPR spectra of (A) 2 mM SLSA in 2 mM BSA solution, (B) 0.8 mM SLSA in 0.8 mM BSA solution, and (C) 0.4 mM SLSA in 0.4 mM BSA solution within a period of time after preparation the samples from 1 minute to 30 minutes.

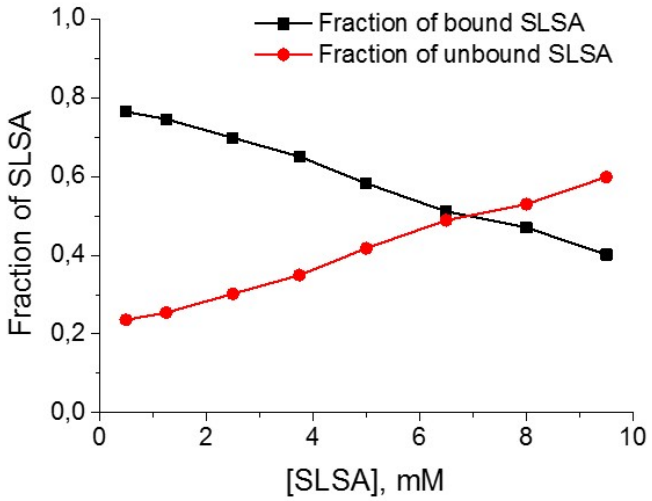

Fig. S6. Fractions of bound (black) and unbound (red) SLSA in 0.5 mM BSA/buffer solution obtained from simulations of their EPR spectra. The concentrations of SLSA are 0.5, 1.2, 2.5, 3.7, 5.0, 6.5, 8.0 and 9.5 mM.

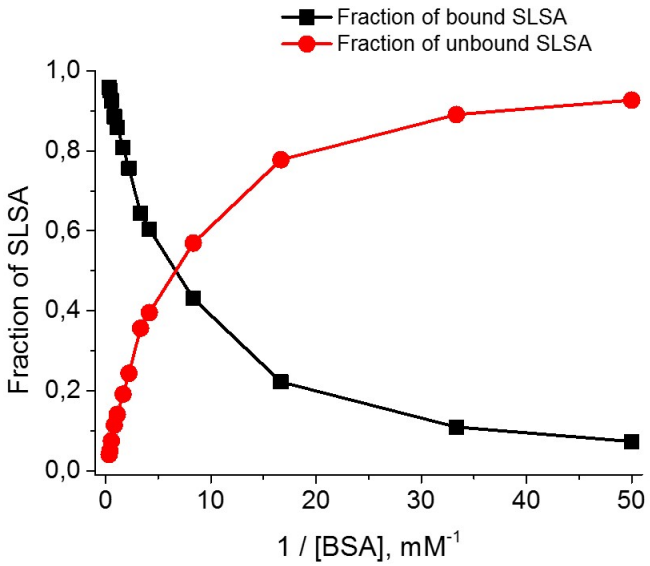

Fig. S7. Fractions of bound (black) and unbound (red) SLSA in different concentrations of BSA (0.02 – 3.00 mM) obtained from simulations of their EPR spectra. The concentration of SLSA was kept constant at 0.6 mM.

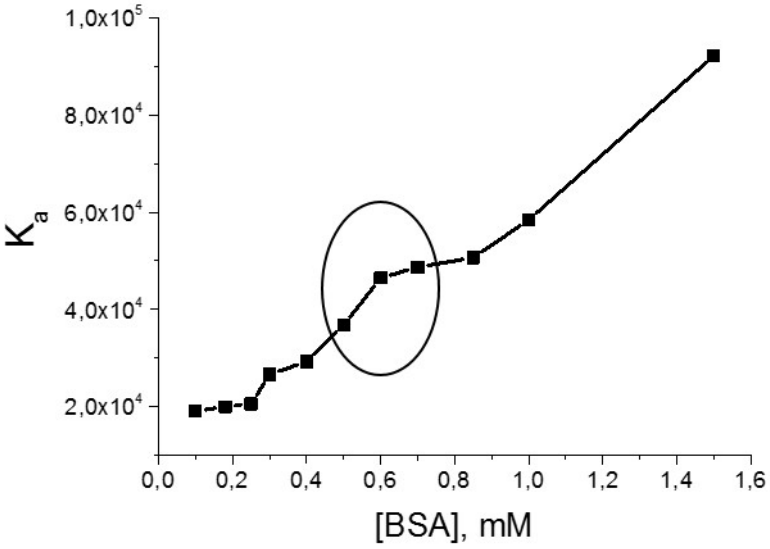

Fig. S8 The curve of calculated K_a versus [BSA] concentration for the SLSA-BSA assembly. The circle shows the concentrations of BSA in the physiological range (0.5 – 0.7 mM BSA).

[BSA], mM	K_a, 10^4 M^{-1}	ΔG, kJ mol^{-1}
0.10	1.91	-24.42
0.18	1.99	-24.54
0.25	2.05	-24.60
0.30	2.66	-25.35
0.40	2.93	-25.48
0.50	3.68	-26.05
0.60	4.65	-26.63
0.70	4.87	-26.74
0.85	5.06	-26.84
1.00	5.84	-27.19
1.50	9.22	-28.32

Table S1. BSA concentrations, association constants (K_a) and binding free energies (ΔG) of SLSA-BSA complexes.