

Supplementary data

Molecular mechanism of tobramycin with human serum albumin for probing the binding interactions: Multi-spectroscopic and computational approaches

Muslim Raza^{1,2*}, Yun Wei¹, Yang Jiang², Aftab Ahmad¹, Saleem Raza³, Sadeeq Ullah¹, Youyou Han², Qudrat Ullah Khan¹, and Yuan Qipeng^{1*}

¹State Key Laboratory of Chemical Resource Engineering, College of Life Science and Technology, Beijing University of Chemical Technology, Beijing, P R China

²Beijing Key Lab of Bioprocess, College of Life Science and Technology, Beijing University of Chemical Technology, 15 Bei San Huan East Road, P. O. Box 53, Beijing 100029, PR China

³State Key Laboratory of Chemical Resource Engineering, College of Materials Science and Engineering, Beijing University of Chemical Technology, Beijing 100029, China

*Correspondence e-mail: yuanqp@mail.buct.edu.cn, raza_chem@upesh.edu.pk

Table S1: Different parameters calculation from the fluorescence data at various temperatures.

T (K)	Slope	Intercept	R ²	KQ (M ⁻¹)	Kq (M ⁻¹ S ⁻¹)
288	0.0545±0.0078	0.590±0.3514	0.95	5.45×10 ⁴ M ⁻¹	8.54×10 ¹² M ⁻¹ S ⁻¹
298	0.0525±0.0008	0.290±0.3653	0.98	5.25×10 ⁴ M ⁻¹	8.22×10 ¹² M ⁻¹ S ⁻¹
308	0.0501±0.0081	0.0094±0.3653	0.90	5.01×10 ⁴ M ⁻¹	7.85×10 ¹² M ⁻¹ S ⁻¹

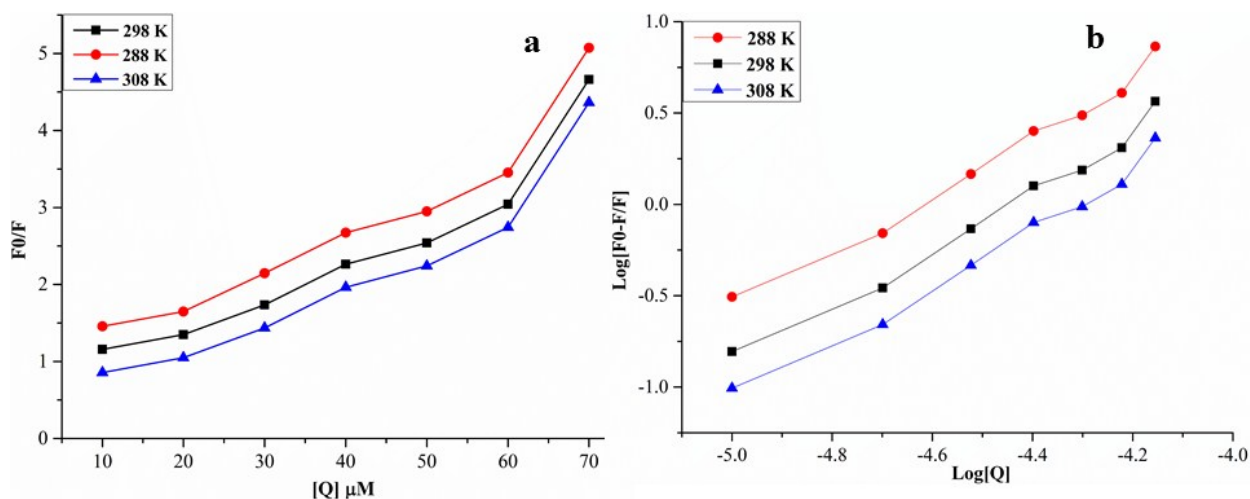


Figure S1: (a) The plot represents modified Stern Volmer equation for calculation of fluorescence intensity at different temperature (288K, 298K and 308K). Double logarithmic plot for calculation of binding constant and other parameters (b).

Table S2. The calculation of binding constant and thermodynamic parameters.

T (K)	R ²	K _s (M ⁻¹)	n	ΔG (Kcal/mol)
288	0.97	1.56×10 ⁶ M ⁻¹	1.02	-6.83
298	0.98	2.06×10 ⁶ M ⁻¹	1	-7.24
308	0.95	1.45×10 ⁶ M ⁻¹	0.6	-7.27

Table S3: Site markers competitive experiment for finding the specific binding site.

Site Markers	KS (M ⁻¹)	n	R ²
HSA-TOB-WAR	1.2× 10 ⁶	0.7	0.99
HSA-TOB-IBU	2.0× 10 ⁶	1	0.98
HSA-TOB-HMN	2.7× 10 ⁶	0.9	0.99

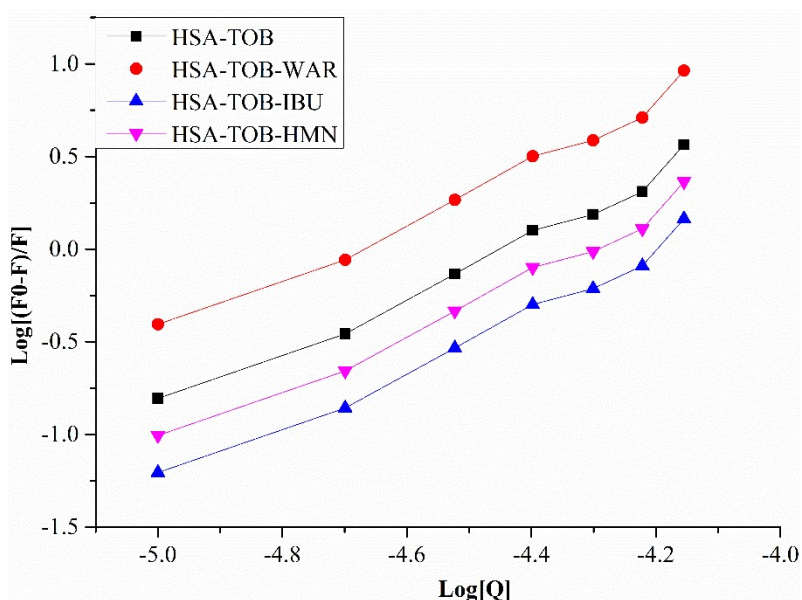


Figure S2: Double logarithmic plot for competitive site probe experiment at 298K. The Ibuprofen, Warfarin and Hemin are represented by the codes IBU WAR and HMN respectively. Three types of markers were used to locate the specific binding site for TOB on HSA.