

Supplementary Information

Multiple Spectroscopic and Theoretical Approaches to Study the Interaction between HSA and the Antiparasitic Drugs: Benznidazole, Metronidazole, Nifurtimox and Megazol

Otávio A. Chaves,^a Romulo C. Ferreira,^a Lorryayne S. da Silva,^a Bruna C. E. de Souza,^a Dari Cesarin-Sobrinho,^a José Carlos Netto-Ferreira,^{a,b} Carlos M. R. Sant'Anna^a and Aurélio B. B. Ferreira^{*a}

^aDepartamento de Química, Universidade Federal Rural do Rio de Janeiro, BR-465 km 7, 23970-000 Seropédica-RJ, Brazil

^bInstituto Nacional de Metrologia, Qualidade e Tecnologia (INMETRO), Divisão de Metrologia Química, 25250-020 Duque de Caxias-RJ, Brazil

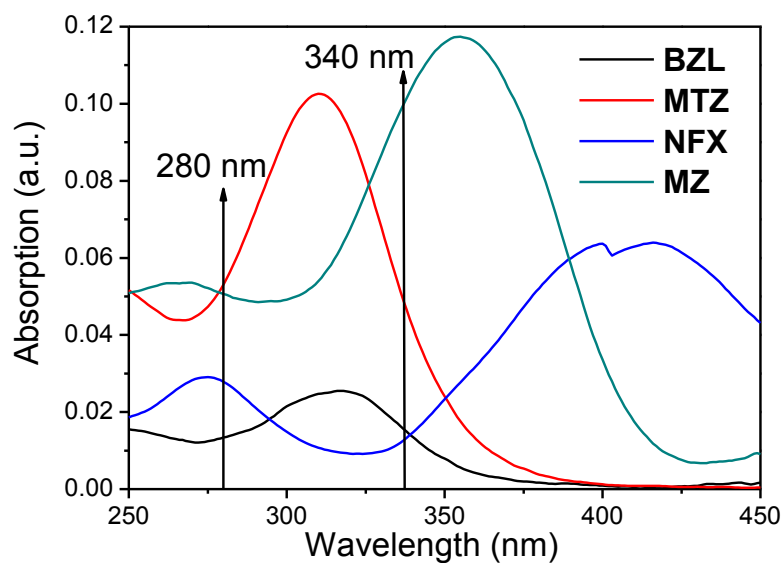


Figure S1. UV-Vis spectra of BZL, MTZ, NFX and MZ in PBS (pH = 7.40) at room temperature. [BZL] = [MTZ] = [NFX] = [MZ] = 1.15×10^{-5} M.

*e-mail: aureliobf@uol.com.br

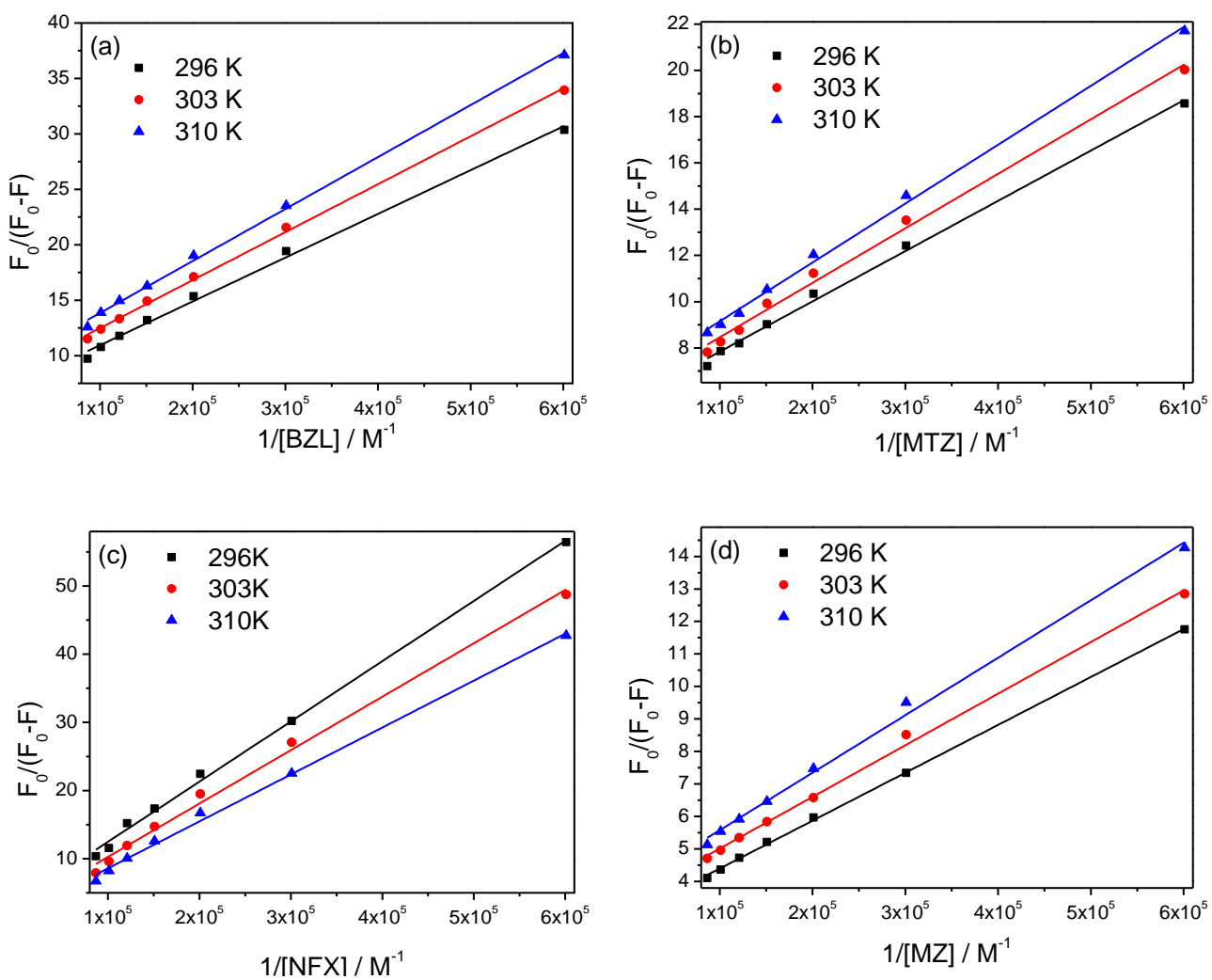


Figure S2. Modified Stern-Volmer plot for the interaction between (a) HSA:BZL; (b) HSA:MTZ; (c) HSA:NFX and (d) HSA:MZ at 296, 303 and 310 K in PBS. $[HSA] = 1.00 \times 10^{-5}$ M; $[BZL] = [MTZ] = [NFX] = [MZ] = 0.17; 0.33; 0.50; 0.66; 0.83; 0.99$ and 1.15×10^{-5} M.

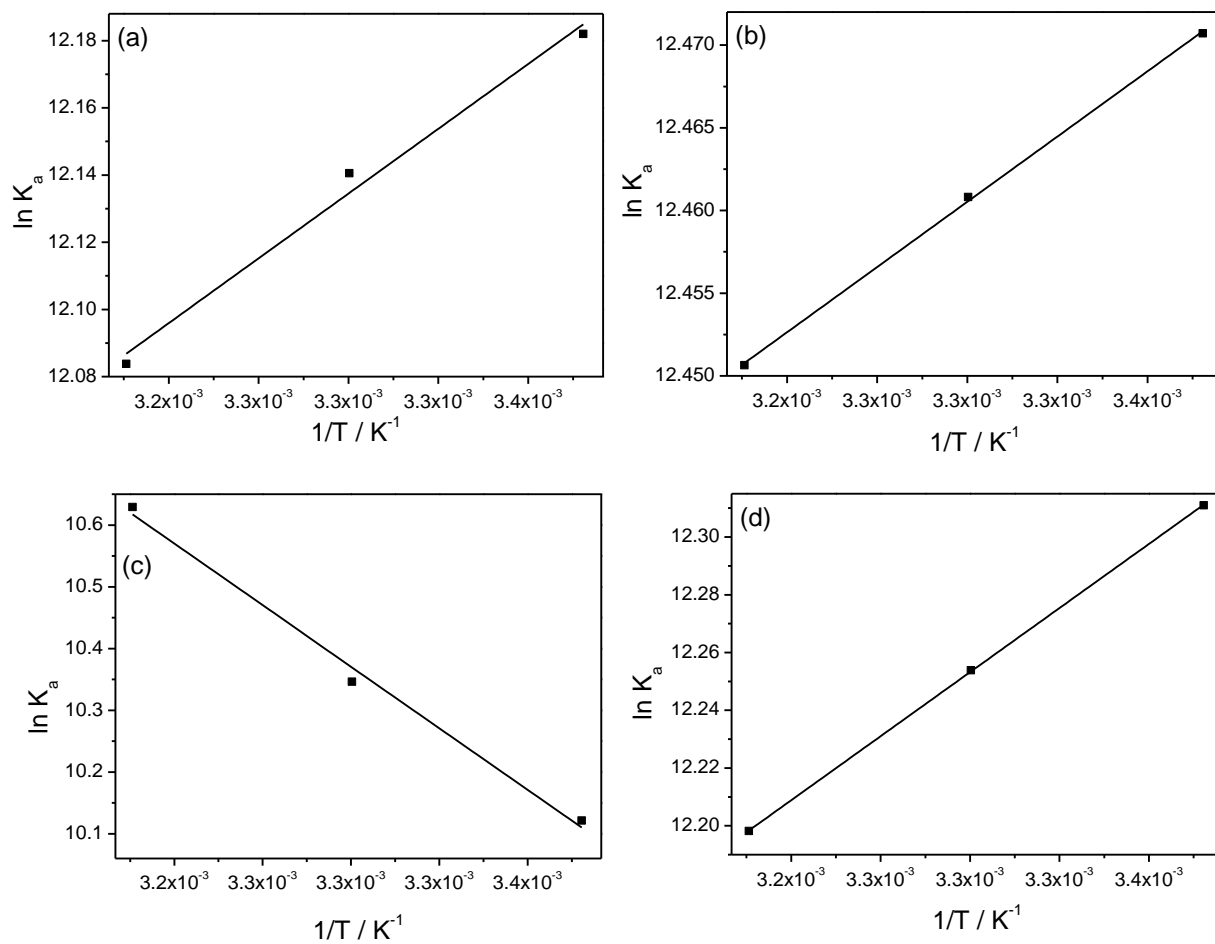


Figure S3. Van't Hoff plot for (a) HSA:BZL; (b) HSA:MTZ; (c) HSA:NFX and (d) HSA:MZ, obtained from the K_a values at 296, 303 and 310 K in PBS.

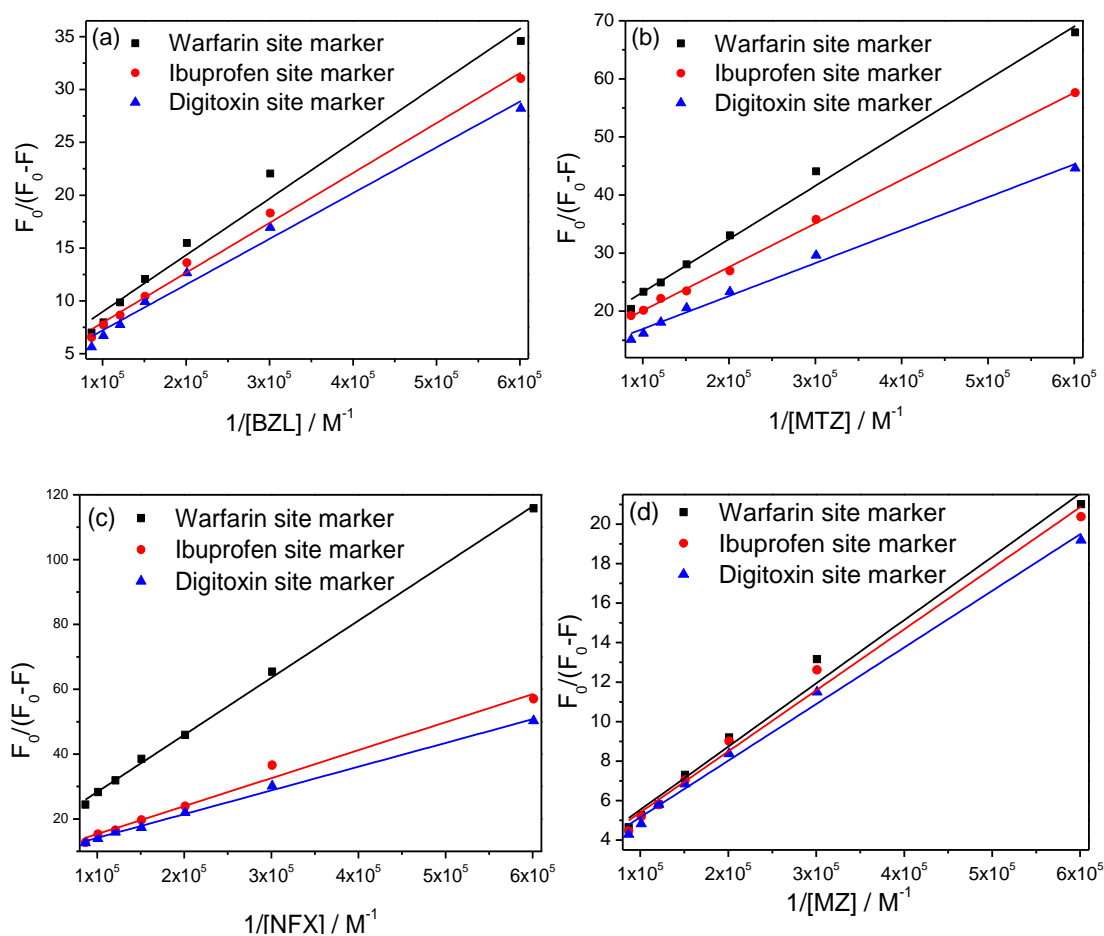


Figure S4. Modified Stern-Volmer plot for the interaction between (a) HSA:BZL; (b) HSA:MTZ; (c) HSA:NFX and (d) HSA:MZ in the presence of site markers warfarin, ibuprofen and digitoxin in PBS at 310 K. $[HSA] = 1.00 \times 10^{-5}$ M; $[BZL] = [MTZ] = [NFX] = [MZ] = 0.17; 0.33; 0.50; 0.66; 0.83; 0.99$ and 1.15×10^{-5} M.