

Supplementary Information

Interaction of β -Carbolines with DNA: Spectroscopic Studies, Correlation with Biological Activity and Molecular Docking

Marina M. Silva,^a Franciele C. Savariz,^b Edeílido F. Silva-Júnior,^a Thiago M. de Aquino,^a
Maria Helena Sarragiotto,^b Josué C. C. Santos^a and Isis M. Figueiredo^{*,a}

^aInstituto de Química e Biotecnologia, Universidade Federal de Alagoas, Campus A.C. Simões,
57072-900 Maceió-AL, Brazil

^bDepartamento de Química, Universidade Estadual de Maringá, 87020-900 Maringá-PR, Brazil

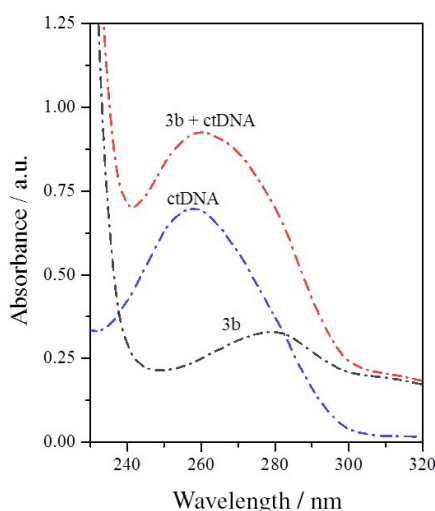


Figure S1. Absorption spectra of **3b** ($10 \mu\text{mol L}^{-1}$), ctDNA ($100 \mu\text{mol L}^{-1}$) and **3b**-ctDNA. Condition: pH = 7.2 (Tris-HCl 50 mmol L^{-1} , 100 mmol L^{-1} NaCl) at 30°C .

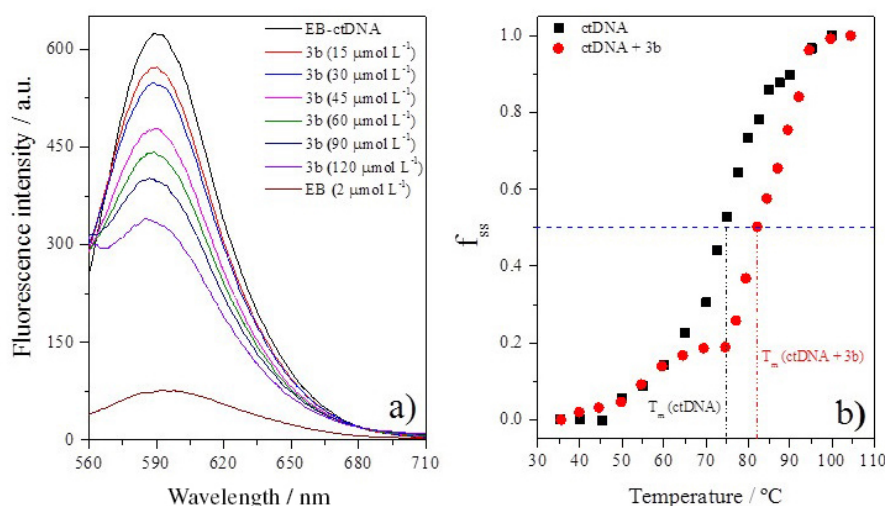


Figure S2. (a) Fluorescence intensity decreasing of EB-DNA system by competition of **3b**. Concentration of EB and ctDNA were 2.0 and $6.0 \mu\text{mol L}^{-1}$, respectively; (b) melting curve of ctDNA at 260 nm in the absence and presence of compound. Condition: pH = 7.2 (Tris-HCl 50 mmol L^{-1} , 100 mmol L^{-1} NaCl) and $\lambda_{\text{exc}} = 525 \text{ nm}$ at 30°C .

*e-mail: figueiredo.isis@gmail.com

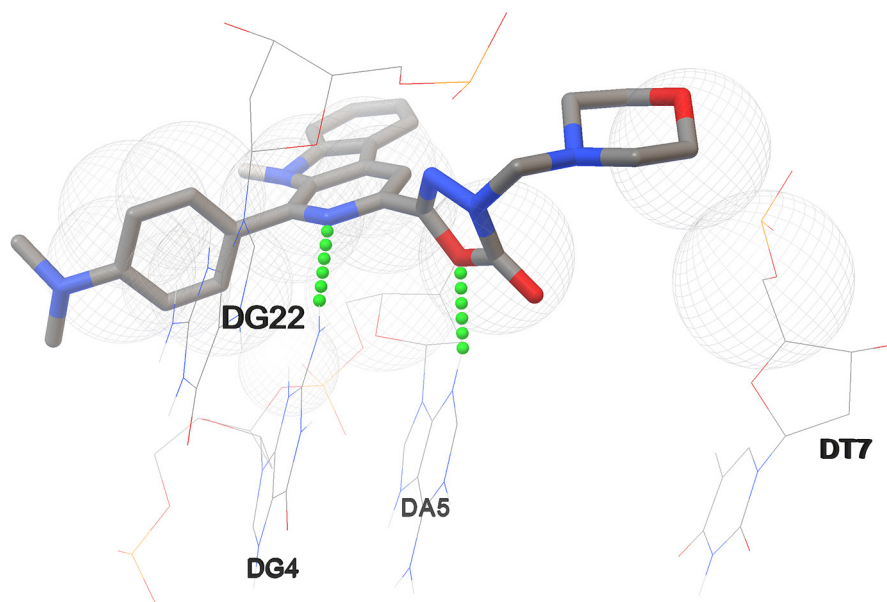
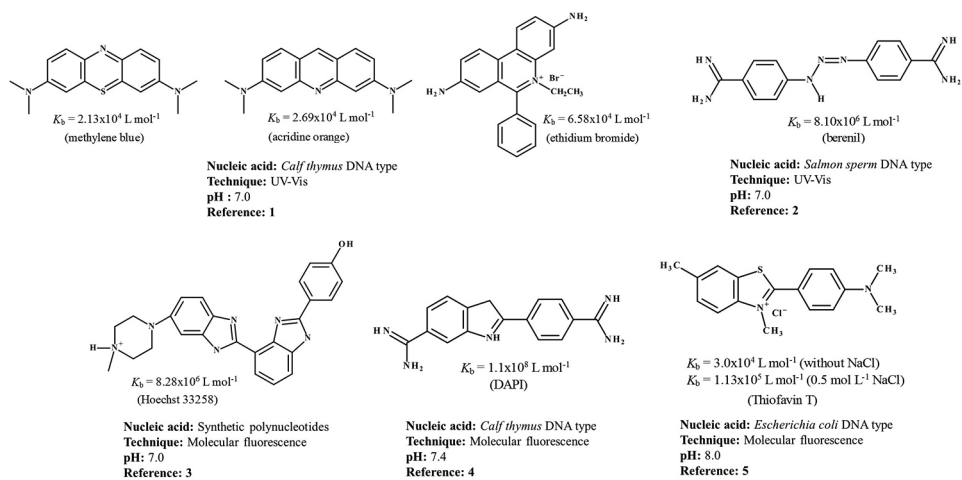
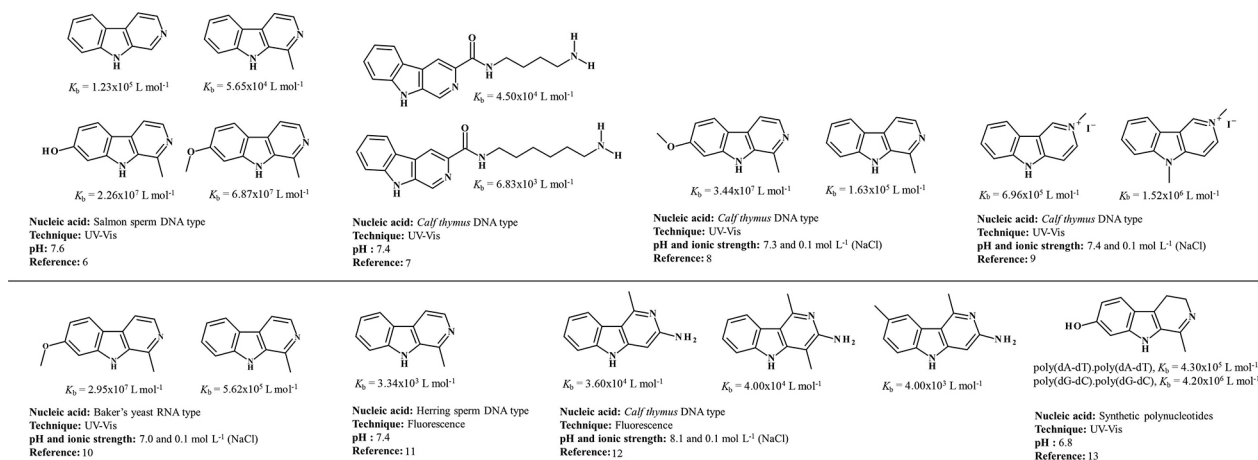


Figure S3. Molecular docked model of **3b** showing significant hydrogen bonds (green dots) and hydrophobic interactions (spheres) with DNA.



Scheme S1. Selected compounds with positive center or amino groups passible of protonation and their interactions parameters with DNA.



Scheme S2. Compilation of some compounds similar to those evaluated and interactions parameters with different nucleic acids.

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