Electronic Supplementary Information

An Experimental and Quantum Chemical Study on the Non-covalent Interactions of a Cyclometallated Rh(III) Complex with DNA and BSA

Roya Esteghamat-Panah,[a] Hossein Farrokhpour,*[a] Hassan Hadadzadeh,*[a] Fatemeh Abyar,[b] and Hadi Amiri Rudbari[c]

[a] *Department of Chemistry, Isfahan University of Technology, Isfahan 84156-83111, Iran*

[b] *Department of Engineering, Ardakan University, Ardakan 89518-95491, Iran*

[c] *Faculty of Chemistry, University of Isfahan, Isfahan 81746-73441, Iran*

*Email: hadad@cc.iut.ac.ir; and h-farrokh@cc.iut.ac.ir

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Table S1 Crystal data and structure refinement for Rh(phpy-$\kappa^2N,C^{2'}$)$_2$(dafone)]PF_6.

Chemical formula	C_{33} H_{22} F_6 N_4 O_2 P Rh
Formula weight	754.43
Temperature (K)	298(2)
Crystal system	Monoclinic
Space group	*P*2(1)/*c*
a (Å)	17.299(4)
b (Å)	13.785(3)
c (Å)	27.191(5)
α (°)	90
β (°)	101.13(3)
γ (°)	90
V (Å^3)	6362(2)
Z	8
D_x (Mg m^{-3})	1.575
F(000)	3024
θ ranges (º)	2.73–25.00
Number of measured reflections	8901
Goodness-of-fit on F^2	0.967
Final *R* indices	R_1 = 0.0732, wR_2 = 0.1852
R indices (all data)	R_1 = 0.1206, wR_2 = 0.2023
Range of *h*, *k*, *l*	−20/20, 0/16, 0/32

1. Type and number of interactions

To analyze the active-site obtained from the docking calculations, the BINANA algorithm was used. This algorithm provides information about the types and numbers of the interactions which contribute to ligand binding. This program determines key binding characteristics like hydrogen bonds and π interactions. The default distances cutoff for the interactions of the type of $\pi - \pi$, cation-π, hydrophobic, T-stacking, and hydrogen bond are 7.5, 6.0, 4.0, 5.0, and 4.0 Å, respectively.[1] Comparison between results obtained from the LIGPLOT+ software and BINANA algorithm shows that there is no hydrogen band in the interaction site for both of DNA and BSA with the Rh(III) complex (Table. S2).

Table S2 Type and number of interactions, calculated by BINANA algorithm, for the complex–DNA and complex–BSA systems.

Target of interactions	H-bond	Hydrophobic contact	$\pi - \pi$ stacking	T-stacking (face-to edge) interactions	Cation-π
DNA	0	12	0	2	0
BSA	0	10	0	0	0

2. Reference

1. J. D. Durrant and J. A. McCammon, *J. Mol. Graphics Modell*, 2011, **29**, 888.

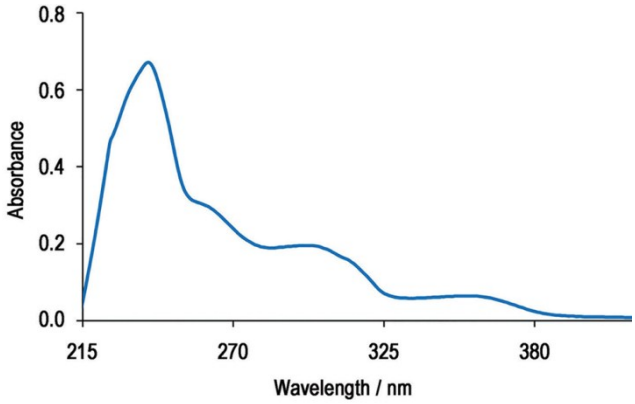

Fig. S1 Electronic spectrum of the Rh(III) complex (5×10^{-6} M in acetonitrile) at room temperature.

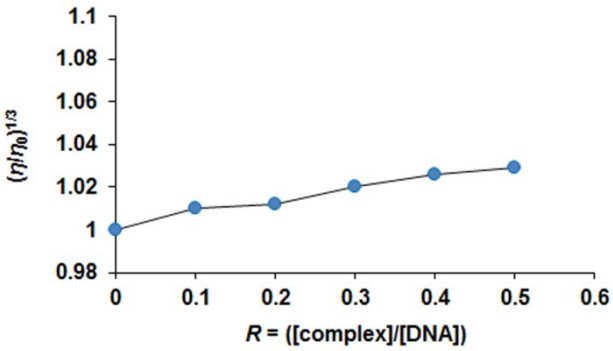

Fig. S2 Relative viscosity $(\eta/\eta_0)^{1/3}$ of DNA (1 mM) in a buffer solution (5 mM Tris–HCl/50 mM NaCl at pH 7.2) in the presence of the Rh(III) complex at increasing amounts (R)

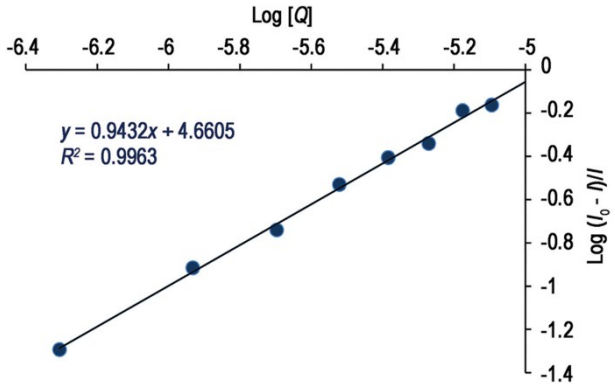

Fig. S3 Determination of the Rh(III) complex–DNA binding constant and the number of the binding sites on DNA at room temperature.

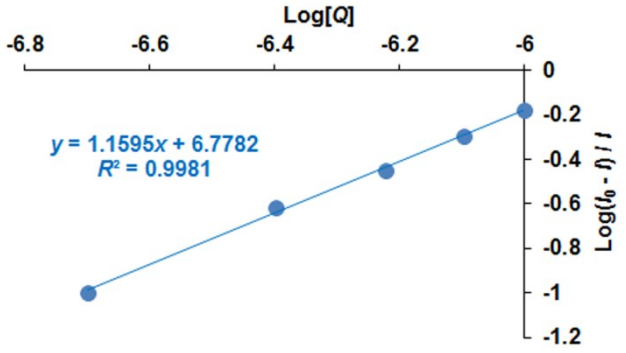

Fig. S4 Determination of the Rh(III) complex–BSA binding constant and the number of the binding sites on BSA at room temperature.

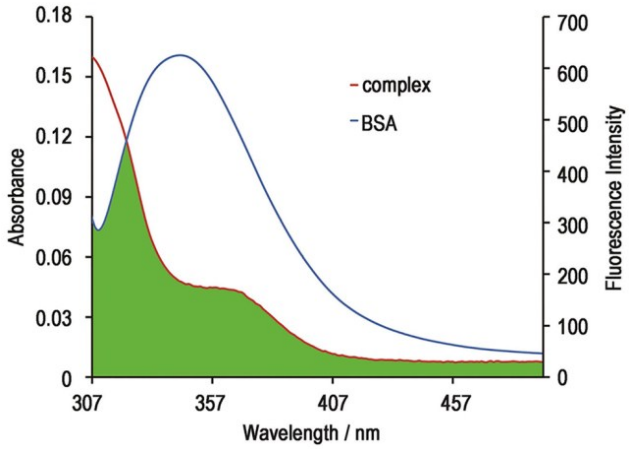

Fig. S5 Spectral overlap of the absorption of the Rh(III) complex with the BSA fluorescence spectrum.