Copper(I) and silver(I) complexes of anthraldehyde thiosemicarbazone: Synthesis, structure elucidation, *in vitro* anti-tuberculosis/cytotoxicity activity and interactions with DNA/HSA

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Supporting Information

Table S1. Binding constants for the interaction of ligand (**H^2L**), copper complexes (**2**, **6** and **8**) and silver complexes (**9** and **10**) with ct-DNA

Compound	K_b ($\times 10^4$ M^{-1})	R
H^2L	1.40	0.9859
2	6.66	0.9129
6	3.06	0.9716
8	3.62	0.9834
9	4.08	0.9830
10	4.60	0.9881

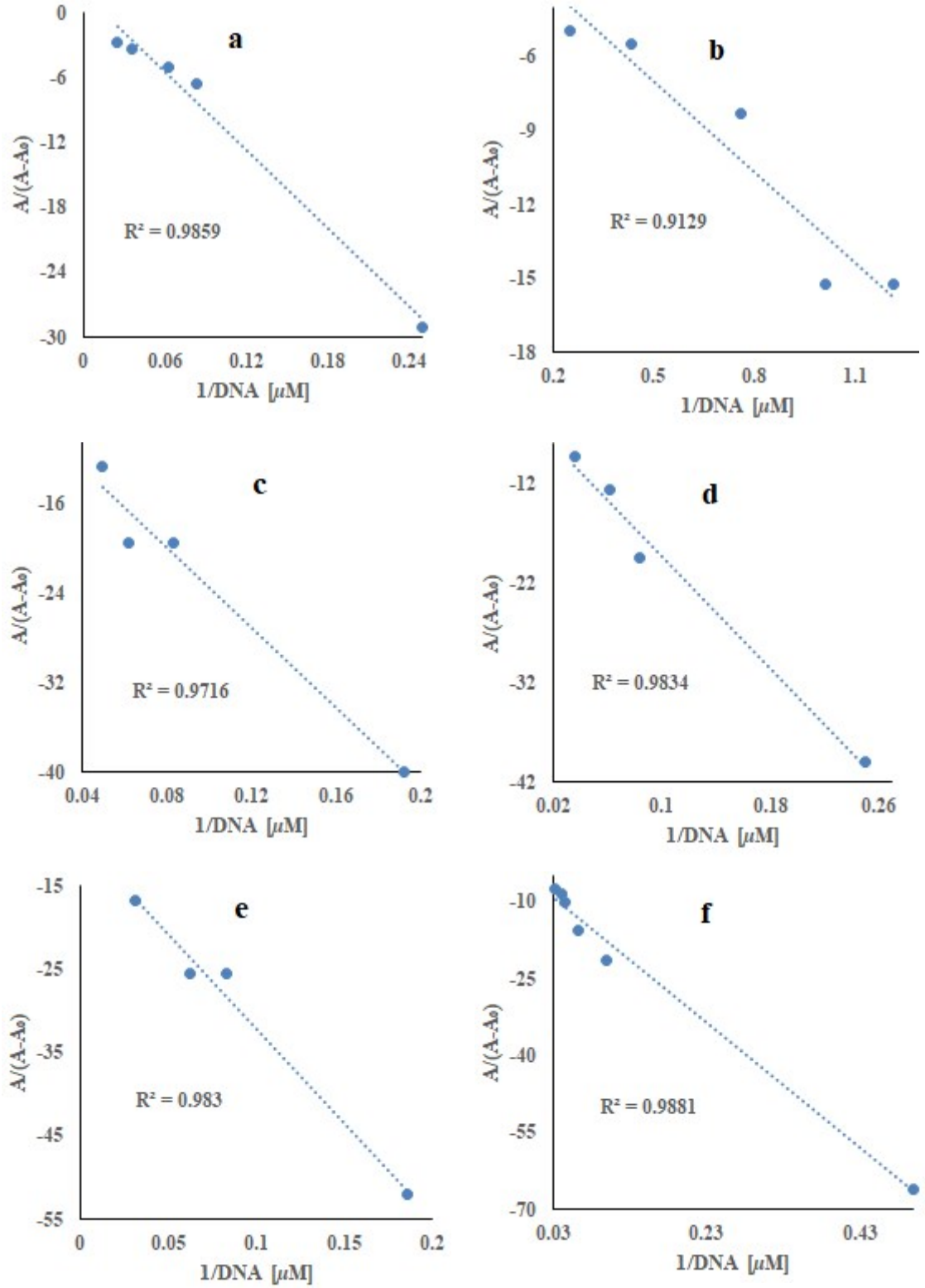
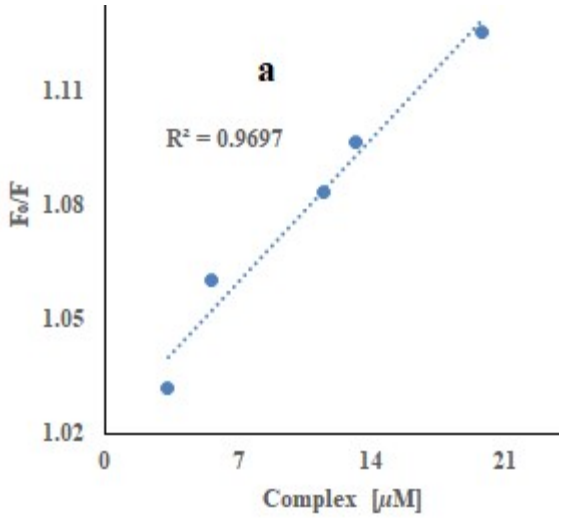
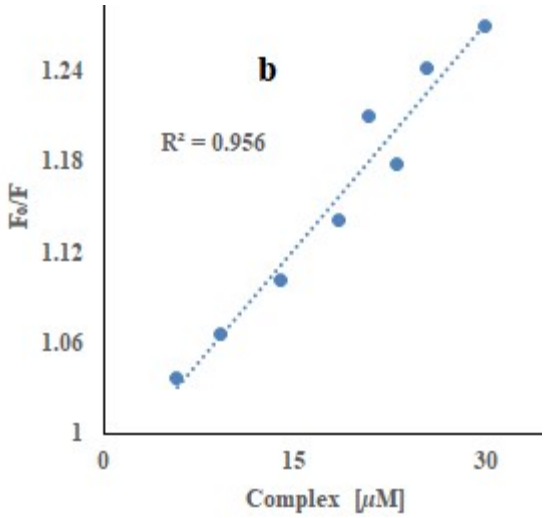
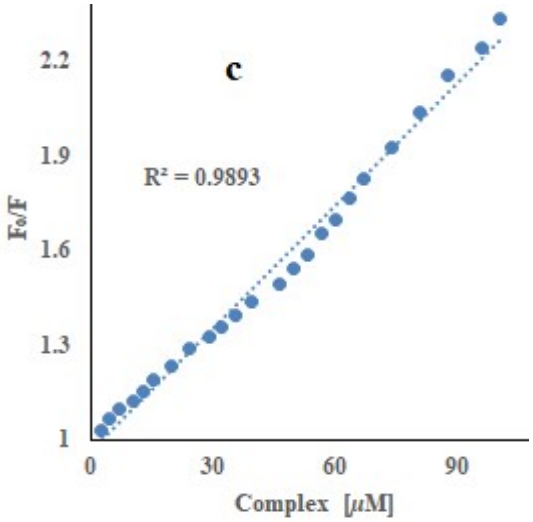
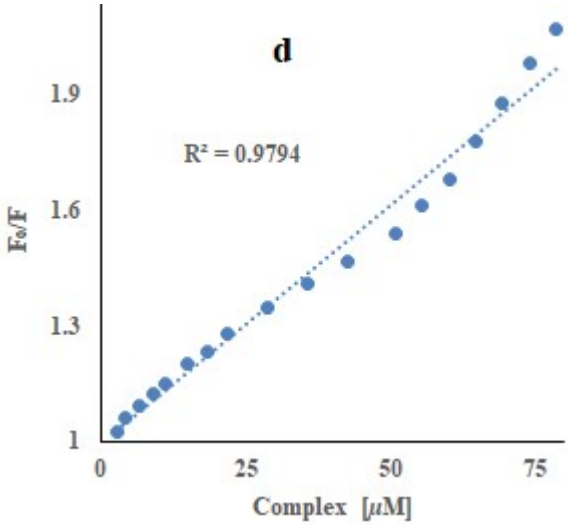


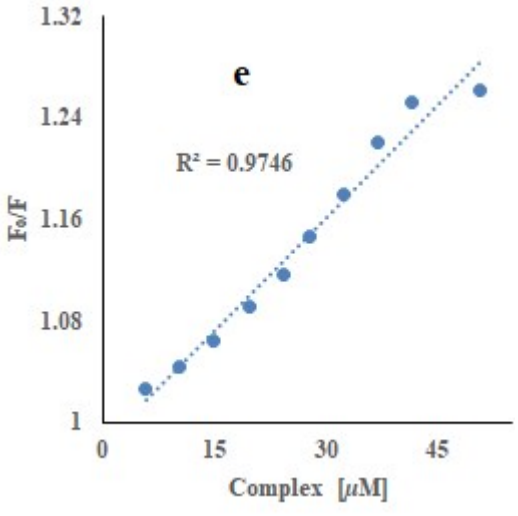
Figure S1. Benesi-Hildebrand plots: {A/(A-A_0) versus 1/DNA [μM]} of absorption spectra of ligand (10 μM) **H^2L** (a); and complexes**2** (b); **6** (c); **8** (d); **9** (e) and **10** (f) with increasing concentrations of ct-DNA.


a
R² = 0.9697
F₀/F
1.11
1.08
1.05
1.02
0
7
14
21
Complex [μM]


b
R² = 0.956
F₀/F
1.24
1.18
1.12
1.06
1
0
15
30
Complex [μM]


c
R² = 0.9893
F₀/F
2.2
1.9
1.6
1.3
1
0
30
60
90
Complex [μM]


d
R² = 0.9794
F₀/F
1.9
1.6
1.3
1
0
25
50
75
Complex [μM]


e
R² = 0.9746
F₀/F
1.32
1.24
1.16
1.08
1
0
15
30
45
Complex [μM]

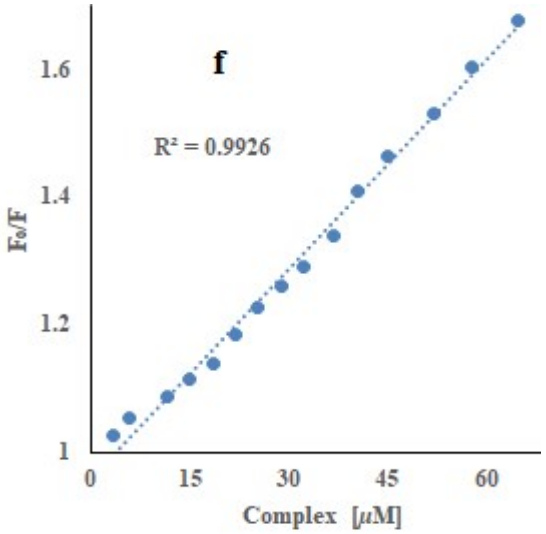
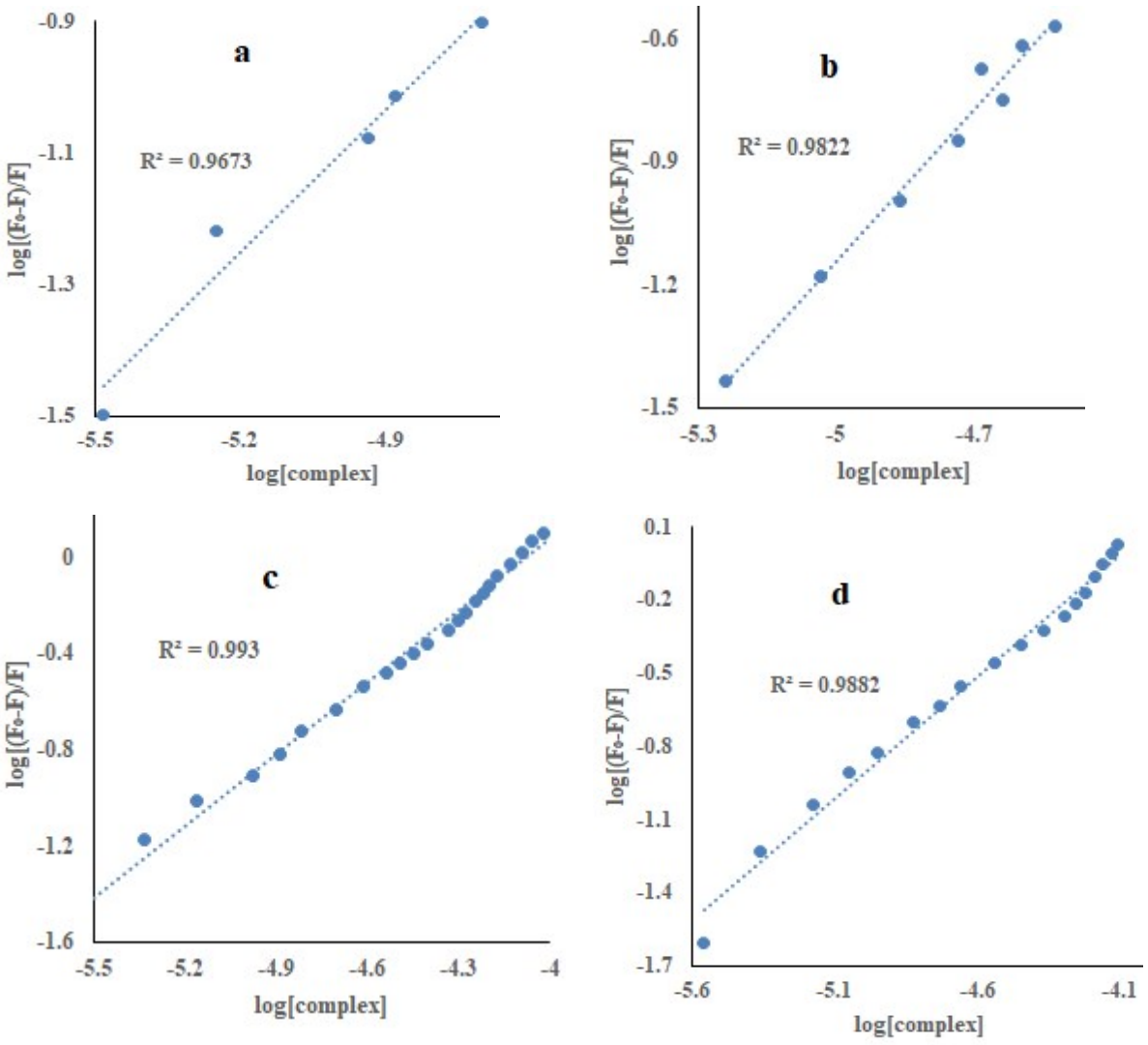
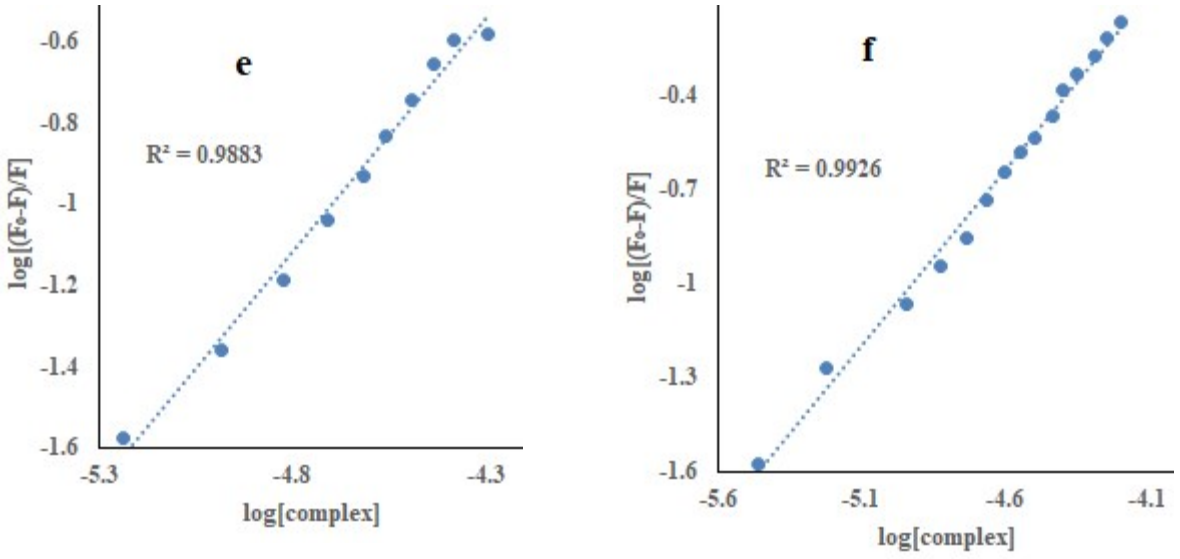

f
R² = 0.9926
F₀/F
1.6
1.4
1.2
1
0
15
30
45
60
Complex [μM]

Figure S2. Stern-Volmer plots {Fo/F versus [complex]} of emission spectra of EB (1 μM) bound to ct-DNA (10 μM) in the absence and increasing concentrations of the ligand **H^2L** (a); and complexes **2** (b); **6** (c); **8** (d); **9** (d) and **10** (f).

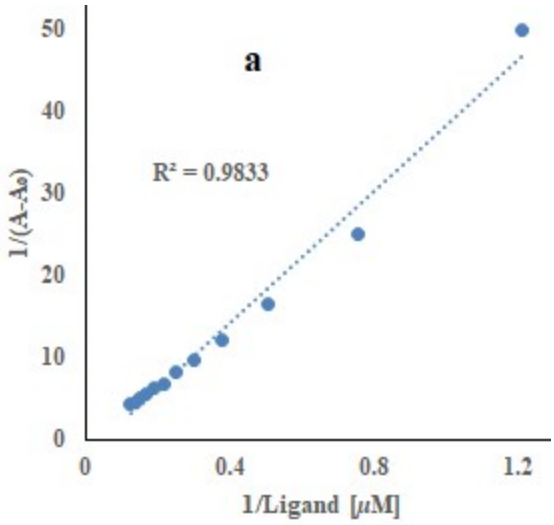


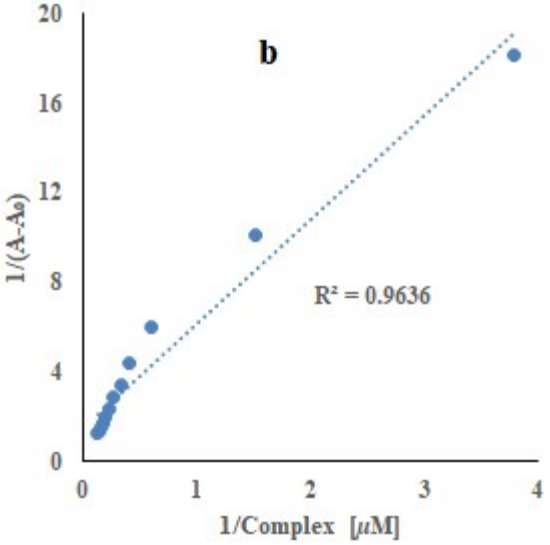


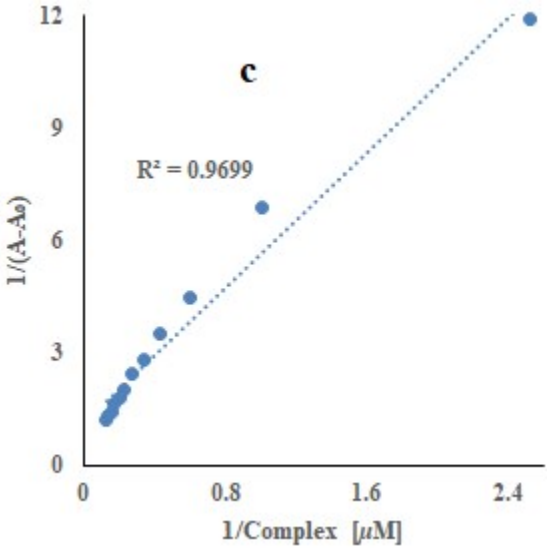
FigureS3. Modified Stern-Volmer plots {log[(Fo-F)/F] versus log[complex]} of emission spectra of EB (1 μM) bound to ct-DNA (10 μM) in the absence and increasing concentrations of the ligand **H^2L** (a); and complexes **2** (b); **6** (c); **8** (d); **9** (d) and **10** (f).

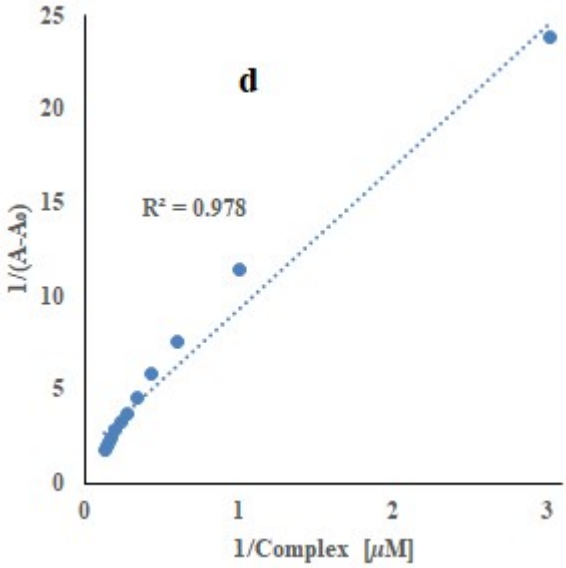
Table S2. Binding constants for the interaction of HSA with ligand (**H^2L**), copper complex (**2**, **6** and **8**) and silver complex (**9** and **10**).

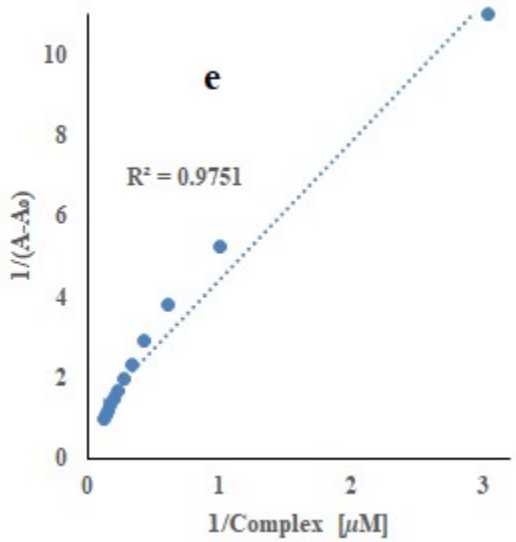
Compound	K_b ($\times 10^5$ M^{-1})	[b]R
H^2L	0.50	0.9833
2	3.28	0.9636
6	2.41	0.9699
8	2.20	0.9780
9	2.82	0.9751
10	3.06	0.9661


a
R² = 0.9833
1/(A-A₀)
1/Ligand [μM]
0
10
20
30
40
50
0
0.4
0.8
1.2


b
R² = 0.9636
1/(A-A₀)
1/Complex [μM]
0
4
8
12
16
20
0
1
2
3
4


c
R² = 0.9699
1/(A-A₀)
1/Complex [μM]
0
3
6
9
12
0
0.8
1.6
2.4


d
R² = 0.978
1/(A-A₀)
1/Complex [μM]
0
5
10
15
20
25
0
1
2
3


e
R² = 0.9751
1/(A-A₀)
1/Complex [μM]
0
2
4
6
8
10
0
1
2
3

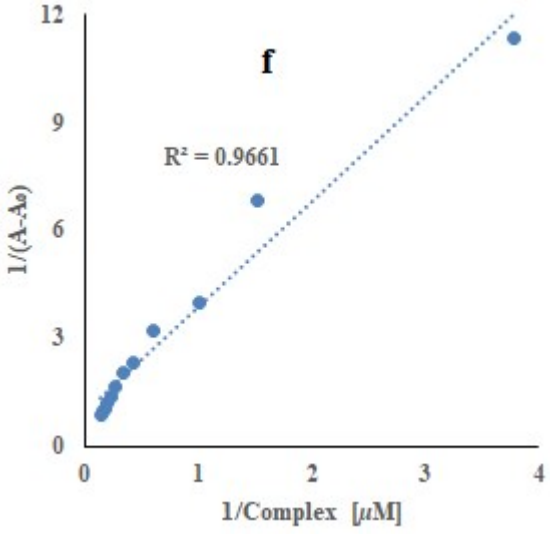
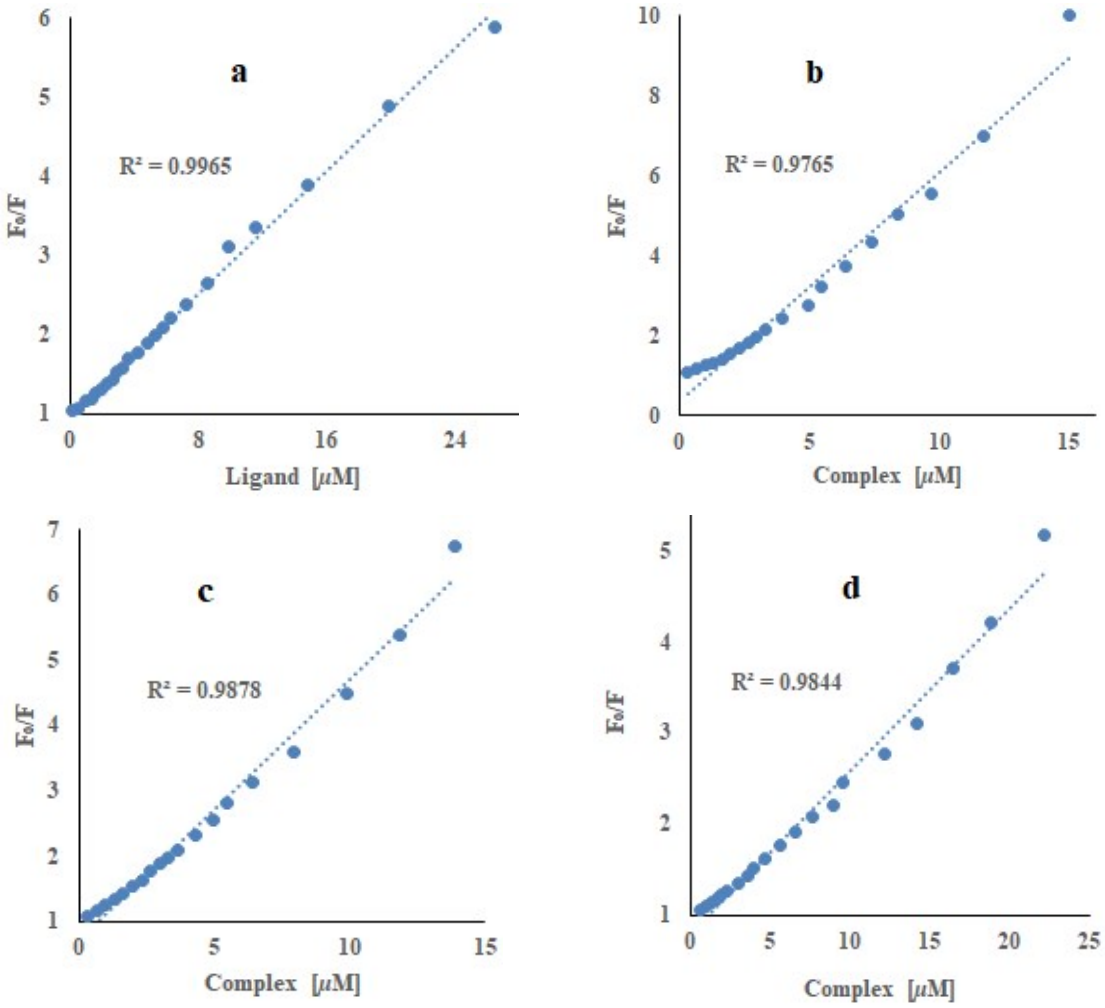

f
R² = 0.9661
1/(A-A₀)
1/Complex [μM]
0
3
6
9
12
0
1
2
3
4

Figure S4. Benesi-Hildebrand plots: {1/(A-A_0) versus 1/complex [μM]} of absorption spectra of HSA (10 μM) with increasing concentrations of ligand **H^2L** (a) and complexes**2** (b); **6** (c); **8** (d); **9** (e) and **10**(f).



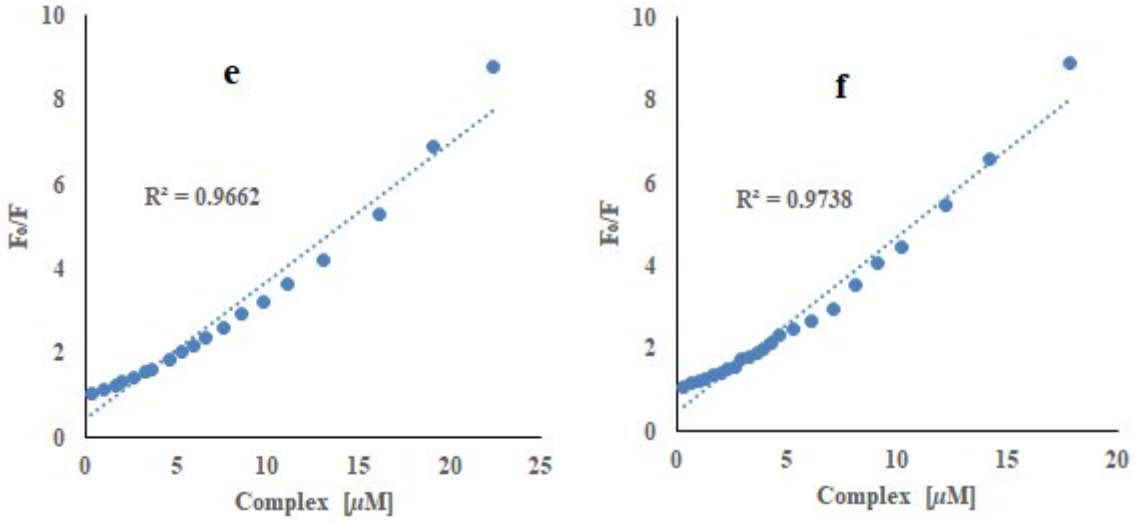
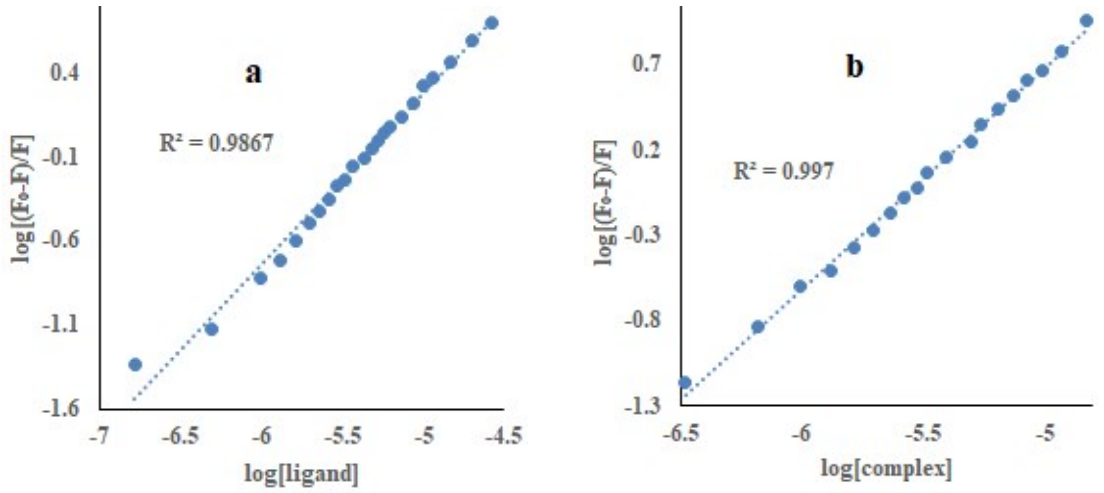
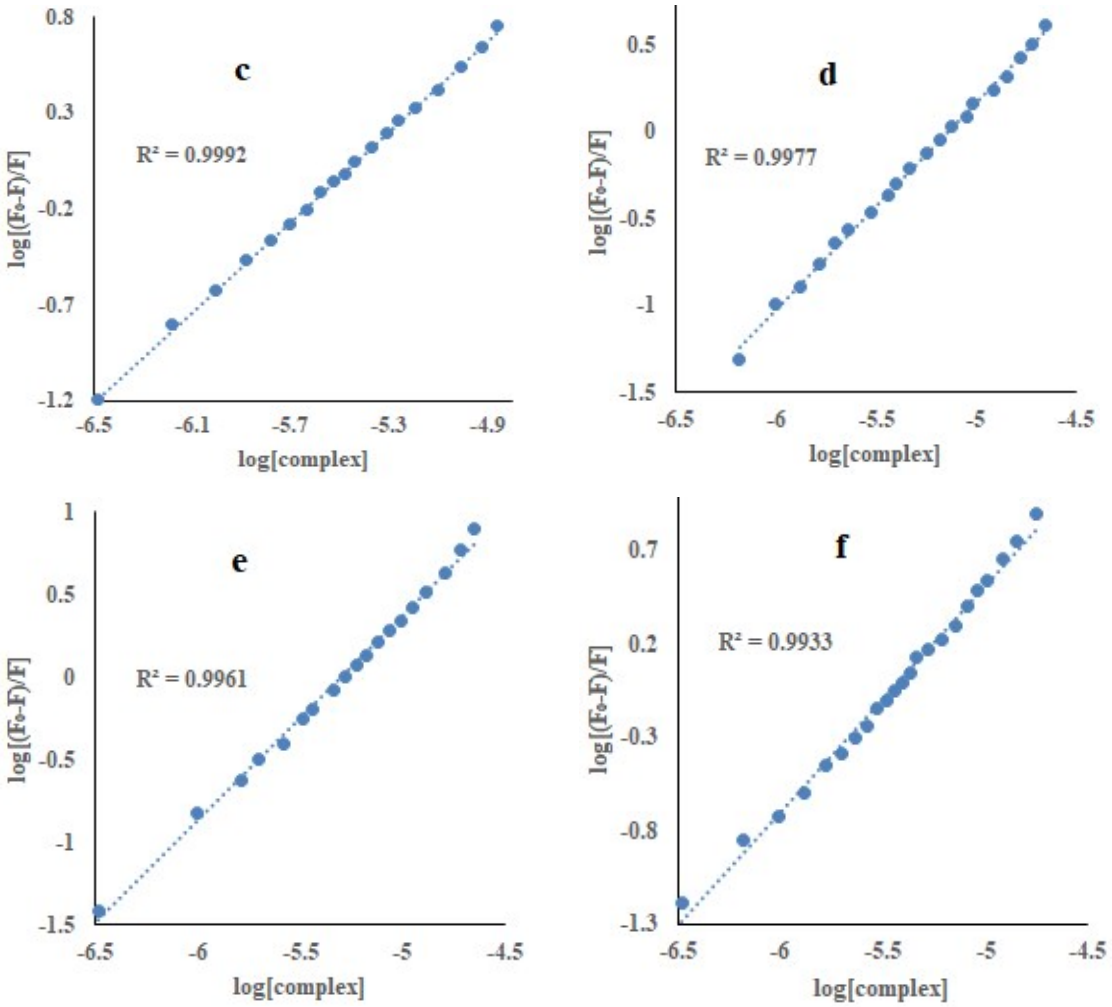


Figure S5. Stern-Volmer plots {Fo/F versus [complex]} of emission spectra of HSA (10 μM) in the absence and increasing concentrations of the ligand **H²L** (a) and complexes**2** (b); **6** (c); **8** (d); **9** (d) and **10** (f).





FigureS6. Modified Stern-Volmer plots {log[(Fo-F)/F] versus log[complex]} of emission spectra of HSA (10 μM) in the absence and increasing concentrations of the ligand **H^2L** (a) and complexes**2** (b); **6** (c); **8** (d); **9** (d) and **10** (f).

Table S3. The docking results based on the binding free energies (kcal/mol) of ligand **H^2L**, and complexes**2** and **6** docked into 1BNA and RMSD from the co-crystallized ligand

Mode	**H^2L**		**2**		**6**	
	Affinity (kcal/mol)	**RMSD (Å)**	**Affinity (kcal/mol)**	**RMSD (Å)**	**Affinity (kcal/mol)**	**RMSD (Å)**
1	-7.1	0.000	-8.1	0.000	-5.9	0.000
2	-6.3	22.560	-8.0	0.568	-5.7	15.175
3	-6.0	2.126	-7.7	0.911	-5.6	15.146
4	-6.0	3.244	-7.7	1.725	-5.6	13.431
5	-5.9	3.651	-7.6	1.003	-5.6	0.430

6	-5.9	22.565	-7.6	0.678	-5.5	0.443
7	-5.9	3.188	-7.6	1.758	-5.5	0.548
8	-5.8	25.636	-7.5	1.769	-5.5	13.999
9	-5.8	3.100	-7.5	1.800	-5.5	0.420

Table S4. The docking results based on the binding free energies (kcal/mol) of complexes**8**, **9** and **10** docked into 1BNA and RMSD from the co-crystallized ligand

Mode	**8**		**9**		**10**	
	Affinity (kcal/mol)	**RMSD (Å)**	**Affinity (kcal/mol)**	**RMSD (Å)**	**Affinity (kcal/mol)**	**RMSD (Å)**
1	-6.4	0.000	-6.4	0.000	-5.9	0.000
2	-6.4	0.346	-6.3	1.966	-5.8	0.756
3	-6.4	0.437	-6.3	0.946	-5.7	2.307
4	-6.4	0.362	-6.3	0.676	-5.7	14.521
5	-6.3	2.180	-6.3	2.016	-5.6	7.969
6	-6.2	2.203	-6.3	0.664	-5.6	2.271
7	-6.2	0.869	-6.3	3.248	-5.6	14.086
8	-6.1	2.126	-6.3	1.946	-5.6	2.365
9	-6.0	3.229	-6.3	6.895	-5.5	14.176

Table S5. The H-bonding of compounds **H^2L**, **2**, **6**, **7**,**8**, **9** and **10** with DNA docked into 1BNA

Comp.	**DNA bases**	**ligand**	**Bond length (Å)**
H^2L	DG-16 (chain B) (O4' of guanine)	NH of ligand (attached with CH_3)	2.49
	DC-15 (chain B) (O2 of cytosine)	NH of ligand (attached with CH_3)	2.75
	DC-15 (chain B) (O2 of cytosine)	NH of ligand (attached with N)	2.53
	DC-11 (chain A) (O2 of cytosine)	NH of ligand (attached with N)	2.89
	DG-16 (chain B) (H3 of guanine)	N of ligand (attached with =CH)	3.03
2	DG-4 (chain A) (H21 of guanine)	N of ligand (attached with =CH)	2.93
	DG-4 (chain A) H22 of guanine)	N of ligand (attached with =CH)	2.66
	DC-23 (chain B) (O4' of cytosine)	NH_2 of ligand	2.13

	DA-6 (chain A) (OP1 of phosphate)	NH_2 of ligand	2.46
6	DC-3 (chain A) (O2 of cytosine)	NH of ligand (attached with CH_3)	2.38
	DG-4 (chain A) (O4' of guanine)	NH of ligand (attached with CH_3)	2.73
8	DG-4 (chain A) (OP4 of phosphate)	NH of ligand (attached with CH_3)	2.14
	DA-17 (chain B) (OP2 of phosphate)	NH of ligand (attached with CH_3)	2.96
9	DG-4 (chain A) (OP2 of phosphate)	NH of ligand (attached with CH_3)	2.13
	DA-17 (chain B) (OP2 of phosphate)	NH of ligand (attached with CH_3)	2.96
	DC-3 (chain A) (OP1 of phosphate)	NH of ligand (attached with CH_3)	3.60
	DA-18 (chain B) (OP2 of phosphate)	NH of ligand (attached with CH_3)	3.75
10	DA-5 (chain A) (H7 of adenine)	Triphenyl ring system	2.90