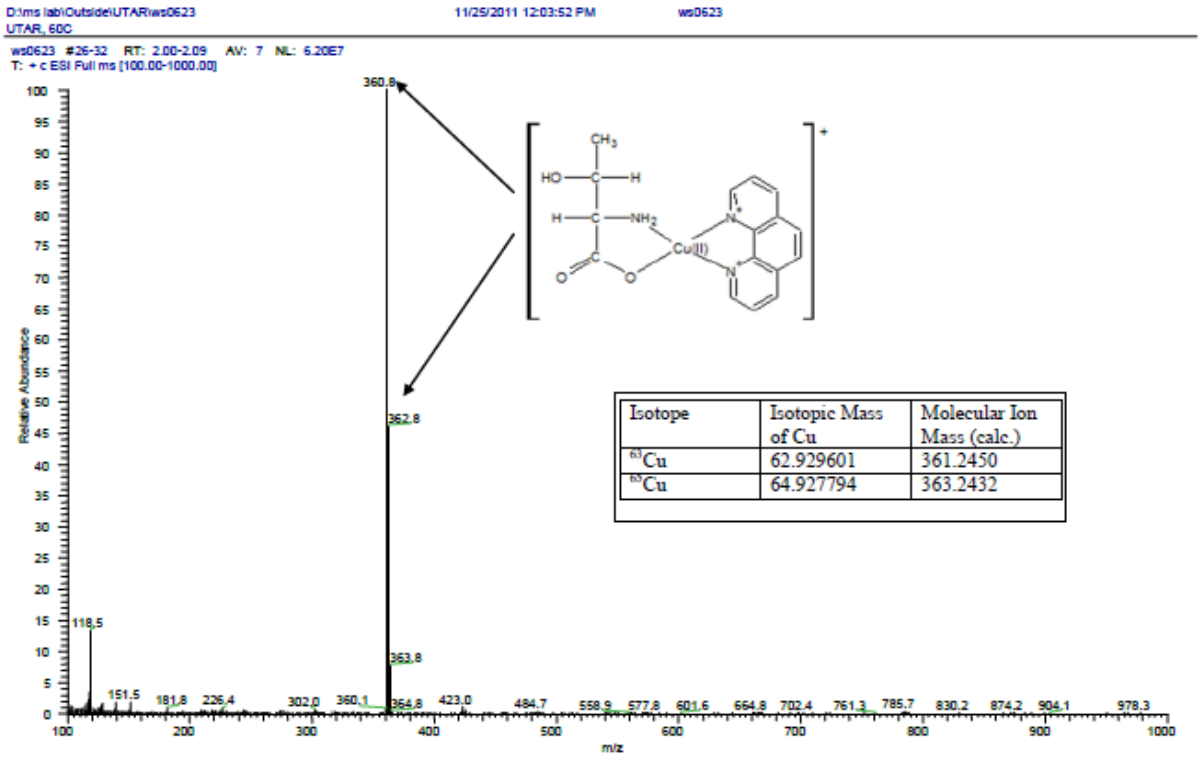
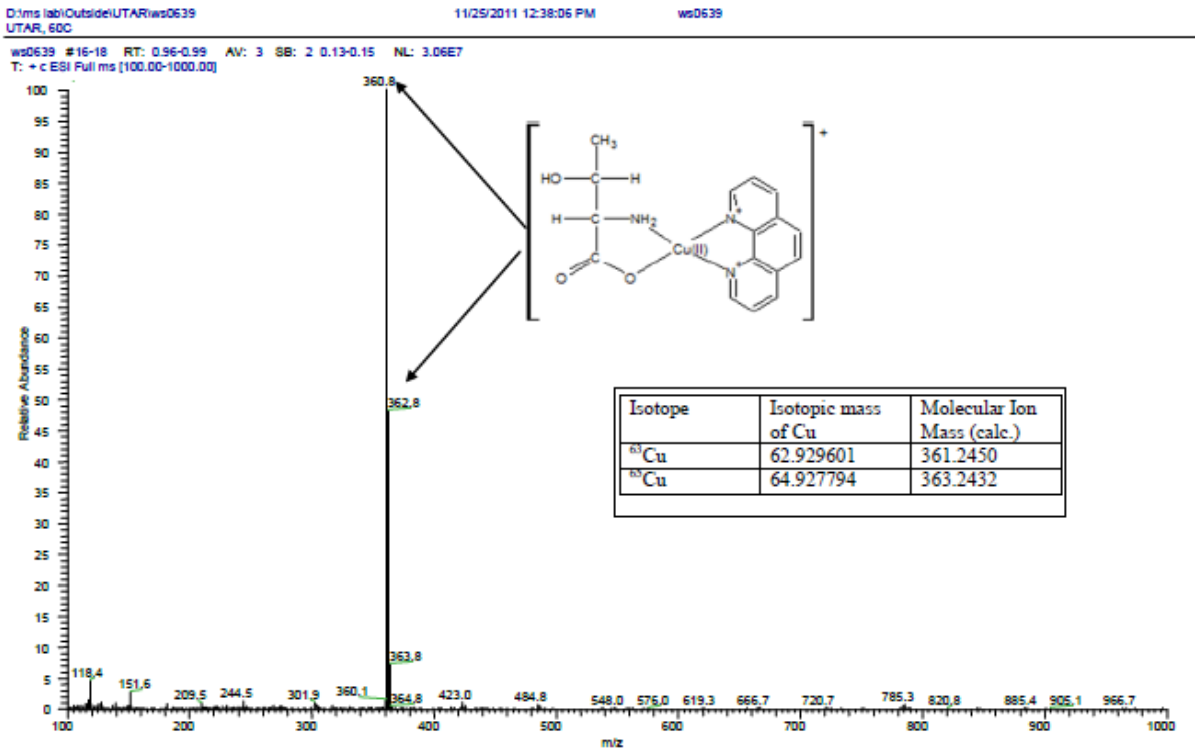
Supplementary Information
Appendix I
(A) ESI-MS spectra (Figs. S1.1-S1.4)

Figure S1.1 ESI-MS spectrum of [Cu(phen)(L-Threo)(H_2O)]NO_3 **1**



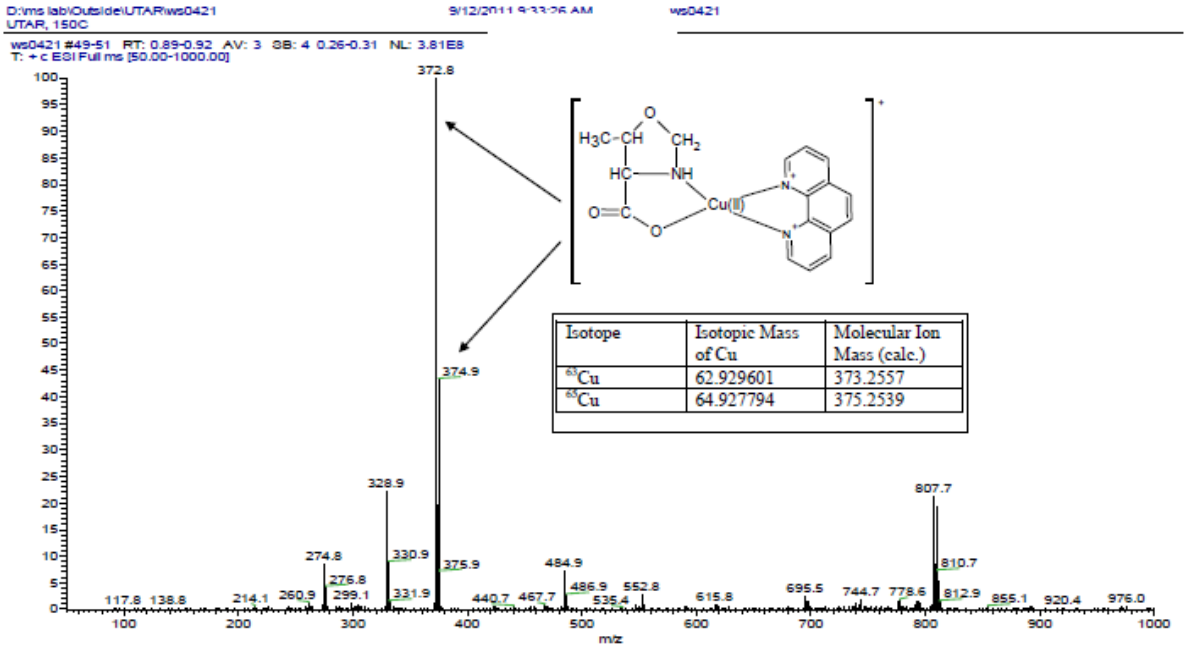
Isotope	Isotopic Mass of Cu	Molecular Ion Mass (calc.)
^{63}Cu	62.929601	361.2450
^{65}Cu	64.927794	363.2432

Figure S1.2 ESI-MS spectrum of [Cu(phen)(D-Threo)(H_2O)]NO_3 **2**



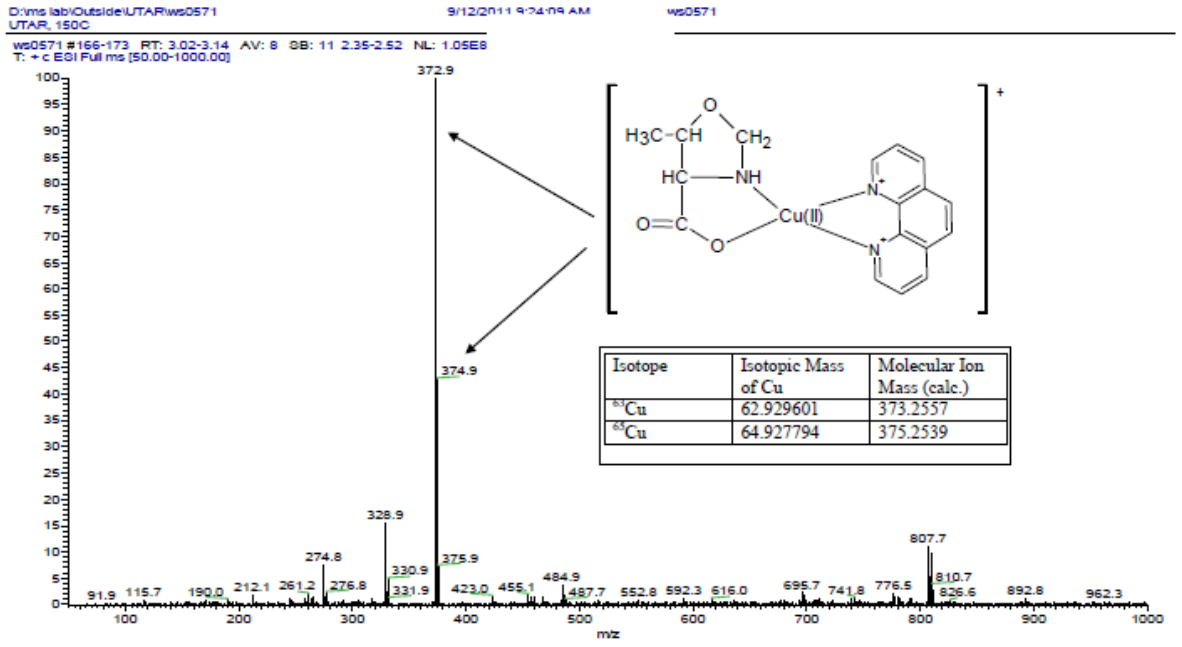
Isotope	Isotopic mass of Cu	Molecular Ion Mass (calc.)
^{63}Cu	62.929601	361.2450
^{65}Cu	64.927794	363.2432

Figure S1.3 ESI-MS spectrum of L-[Cu(phen)(5MeOCA)(H_2O)]NO_3 3

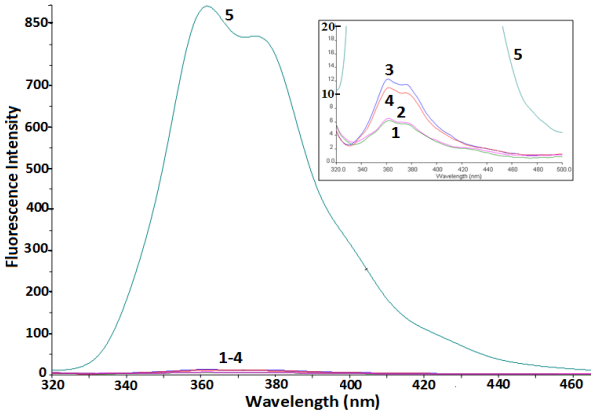


Isotope	Isotopic Mass of Cu	Molecular Ion Mass (calc.)
^{63}Cu	62.929601	373.2557
^{65}Cu	64.927794	375.2539

Figure 1.4 ESI-MS spectrum of D-[Cu(phen)(5MeOCA)(H_2O)]NO_3 4



Isotope	Isotopic Mass of Cu	Molecular Ion Mass (calc.)
^{63}Cu	62.929601	373.2557
^{65}Cu	64.927794	375.2539



Supplementary Fig. S2 Fluorescence spectra of $1x10^{-5}$ M **1** – **5** in water-methanol (1:1 v/v). Insert shows clearly the FL spectra of **1** – **4**.

(B) Restriction Enzyme inhibition by $CuCl_2$, [Cu(phen)Cl_2], and copper(II) complexes **1-4** (Figs. S3.1-S3.6)

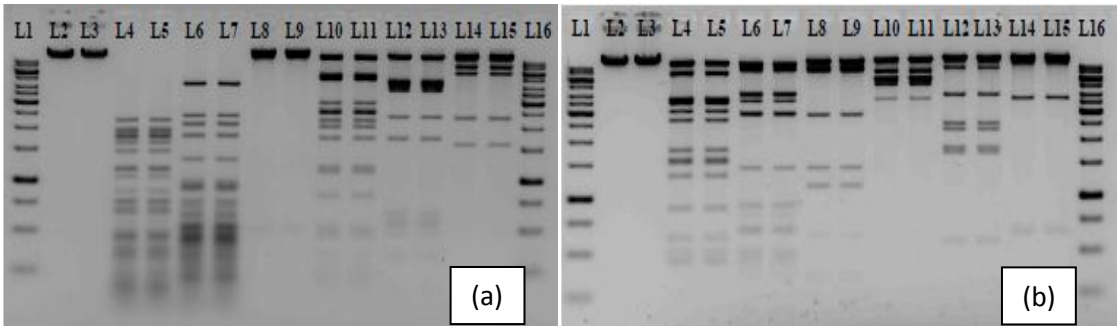


Figure S3.1 RE inhibition by $CuCl_2$. Electrophoresis results of incubating λ DNA (0.5 μg/μL) with 5 unit of restriction enzyme in the presence or absence of 50 μM $CuCl_2$ for 2 hours at 37ºC.
(a) Lane 1, 1kb DNA ladder; Lane 2, λ DNA alone (0.5 μg); Lane 3, λ DNA + 50 μM $CuCl_2$; Lane 4, λ DNA + 5 unit Tsp 509I (control); Lane 5, λ DNA + 5 unit Tsp 509I + 50 μM $CuCl_2$; Lane 6, λ DNA + 5 unit Hae III (control); Lane 7, λ DNA + 5 unit Hae III + 50 μM $CuCl_2$; Lane 8, λ DNA + 5 unit Sal I (control); Lane 9, λ DNA + 5 unit Sal I + 50 μM $CuCl_2$; Lane 10, λ DNA + 5 unit Pst I (control); Lane 11, λ DNA + 5 unit Pst I + 50 μM $CuCl_2$; Lane 12, λ DNA + 5 unit Pvu II (control); Lane 13, λ DNA + 5 unit Pvu II + 50 μM $CuCl_2$; Lane 14, λ DNA + 5 unit Sca I (control); Lane 15, λ DNA + 5 unit Sca I + 50 μM $CuCl_2$; Lane 16, 1kb DNA ladder.
(b) Lane 1, 1kb DNA ladder; Lane 2, λ DNA alone (0.5 μg); Lane 3, λ DNA + 50 μM $CuCl_2$; Lane 4, λ DNA + 5 unit Ssp I (control); Lane 5, λ DNA + 5 unit Ssp I + 50 μM $CuCl_2$; Lane 6, λ DNA + 5 unit Ase I (control); Lane 7, λ DNA + 5 unit Ase I + 50 μM $CuCl_2$; Lane 8, λ DNA + 5 unit Mun I (control); Lane 9, λ DNA + 5 unit Mun I + 50 μM $CuCl_2$; Lane 10, λ DNA + 5 unit EcoR I (control); Lane 11, λ DNA + 5 unit EcoR I + 50 μM metal salt; Lane 12, λ DNA + 5 unit NdeI (control); Lane 13, λ DNA + 5 unit NdeI + 50 μM $CuCl_2$; Lane 14, λ DNA + 5 unit Bst 11071 (control); Lane 15, λ DNA + 5 unit Bst 11071 + 50 μM $CuCl_2$; Lane 16, 1kb DNA ladder.

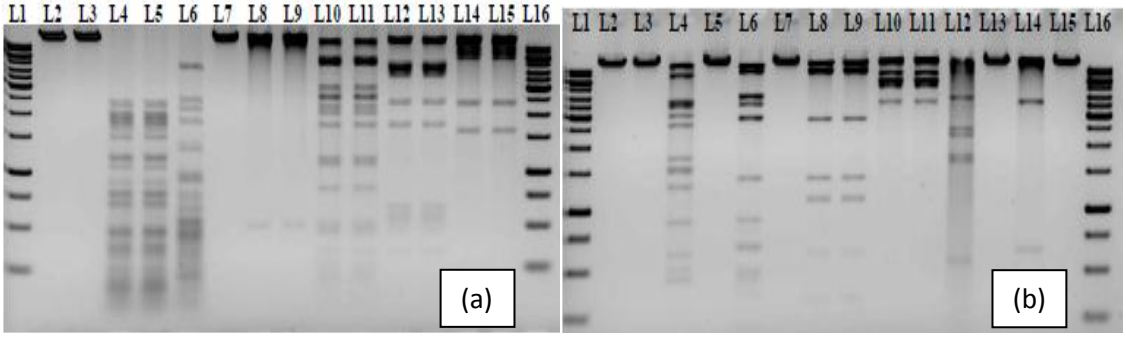


Figure S3.2 RE inhibition by [Cu(phen)Cl_2]. Electrophoresis results of incubating λ DNA (0.5 μg/μL) with 5 unit of restriction enzyme in the presence or absence of 50 μM [Cu(phen)Cl_2] for 2 hours at 37ºC.

(a) Lane 1, 1kb DNA ladder; Lane 2, λ DNA alone (0.5 μg); Lane 3, λ DNA + 50 μM [Cu(phen)Cl_2]; Lane 4, λ DNA + 5 unit Tsp 509I (control); Lane 5, λ DNA + 5 unit Tsp 509I + 50 μM [Cu(phen)Cl_2]; Lane 6, λ DNA + 5 unit Hae III (control); Lane 7, λ DNA + 5 unit Hae III + 50 μM [Cu(phen)Cl_2]; Lane 8, λ DNA + 5 unit Sal I (control); Lane 9, λ DNA + 5 unit Sal I + 50 μM [Cu(phen)Cl_2]; Lane 10, λ DNA + 5 unit Pst I (control); Lane 11, λ DNA + 5 unit Pst I + 50 μM [Cu(phen)Cl_2]; Lane 12, λ DNA + 5 unit Pvu II (control); Lane 13, λ DNA + 5 unit Pvu II + 50 μM [Cu(phen)Cl_2]; Lane 14, λ DNA + 5 unit Sca I (control); Lane 15, λ DNA + 5 unit Sca I + 50 μM [Cu(phen)Cl_2]; Lane 16, 1kb DNA ladder.

(b) Lane 1, 1kb DNA ladder; Lane 2, λ DNA alone (0.5 μg); Lane 3, λ DNA + 50 μM [Cu(phen)Cl_2]; Lane 4, λ DNA + 5 unit Ssp I (control); Lane 5, λ DNA + 5 unit Ssp I + 50 μM [Cu(phen)Cl_2]; Lane 6, λ DNA + 5 unit Ase I (control); Lane 7, λ DNA + 5 unit Ase I + 50 μM [Cu(phen)Cl_2]; Lane 8, λ DNA + 5 unit Mun I (control); Lane 9, λ DNA + 5 unit Mun I + 50 μM [Cu(phen)Cl_2]; Lane 10, λ DNA + 5 unit EcoR I (control); Lane 11, λ DNA + 5 unit EcoR I + 50 μM [Cu(phen)Cl_2]; Lane 12, λ DNA + 5 unit NdeI (control); Lane 13, λ DNA + 5 unit NdeI + 50 μM [Cu(phen)Cl_2]; Lane 14, λ DNA + 5 unit Bst 11071 (control); Lane 15, λ DNA + 5 unit Bst 11071 + 50 μM [Cu(phen)Cl_2]; Lane 16, 1kb DNA ladder.

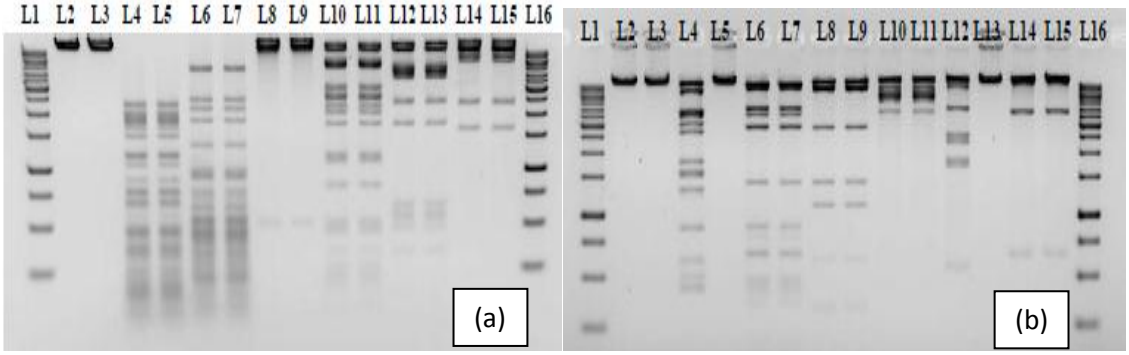


Figure S3.3 RE inhibition by **1.** Electrophoresis results of incubating λ DNA (0.5 μg/μL) with 5 unit of restriction enzyme in the presence or absence of 50 μM **1** for 2 hours at 37ºC.
(a) Lane 1, 1kb DNA ladder; Lane 2, λ DNA alone (0.5 μg); Lane 3, λ DNA + 50 μM **1**; Lane 4, λ DNA + 5 unit Tsp 509I (control); Lane 5, λ DNA + 5 unit Tsp 509I + 50 μM **1**; Lane 6, λ DNA + 5 unit Hae III (control); Lane 7, λ DNA + 5 unit Hae III + 50 μM **1**; Lane 8, λ DNA + 5 unit Sal I (control); Lane 9, λ DNA + 5 unit Sal I + 50 μM **1**; Lane 10, λ DNA + 5 unit Pst I (control); Lane 11, λ DNA + 5 unit Pst I + 50 μM **1**; Lane 12, λ DNA + 5 unit Pvu II (control); Lane 13, λ DNA + 5 unit Pvu II + 50 μM **1**; Lane 14, λ DNA + 5 unit Sca I (control); Lane 15, λ DNA + 5 unit Sca I + 50 μM **1**; Lane 16, 1kb DNA ladder.
(b) Lane 1, 1kb DNA ladder; Lane 2, λ DNA alone (0.5 μg); Lane 3, λ DNA + 50 μM **1**; Lane 4, λ DNA + 5 unit Ssp I (control); Lane 5, λ DNA + 5 unit Ssp I + 50 μM **1**; Lane 6, λ DNA + 5 unit Ase I (control); Lane 7, λ DNA + 5 unit Ase I + 50 μM **1**; Lane 8, λ DNA + 5 unit Mun I (control); Lane 9, λ DNA + 5 unit Mun I + 50 μM **1**; Lane 10, λ DNA + 5 unit EcoR I (control); Lane 11, λ DNA + 5 unit EcoR I + 50 μM **1**; Lane 12, λ DNA + 5 unit NdeI (control); Lane 13, λ DNA + 5 unit NdeI + 50 μM **1**; Lane 14, λ DNA + 5 unit Bst 11071 (control); Lane 15, λ DNA + 5 unit Bst 11071 + 50 μM **1**; Lane 16, 1kb DNA ladder.

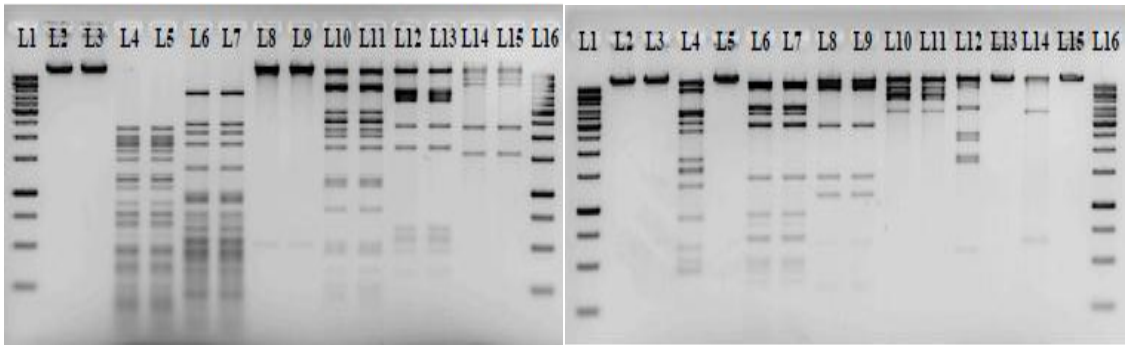


Figure S3.4 RE inhibition by **2**.

Electrophoresis results of incubating λ DNA (0.5 μg/μL) with 5 unit of restriction enzyme in the presence or absence of 50 μM **2** for 2 hours at 37ºC.

(a) Lane 1, 1kb DNA ladder; Lane 2, λ DNA alone (0.5 μg); Lane 3, λ DNA + 50 μM **2**; Lane 4, λ DNA + 5 unit Tsp 509I (control); Lane 5, λ DNA + 5 unit Tsp 509I + 50 μM **2**; Lane 6, λ DNA + 5 unit Hae III (control); Lane 7, λ DNA + 5 unit Hae III + 50 μM **2**; Lane 8, λ DNA + 5 unit Sal I (control); Lane 9, λ DNA + 5 unit Sal I + 50 μM **2**; Lane 10, λ DNA + 5 unit Pst I (control); Lane 11, λ DNA + 5 unit Pst I + 50 μM **2**; Lane 12, λ DNA + 5 unit Pvu II (control); Lane 13, λ DNA + 5 unit Pvu II + 50 μM **2**; Lane 14, λ DNA + 5 unit Sca I (control); Lane 15, λ DNA + 5 unit Sca I + 50 μM **2**; Lane 16, 1kb DNA ladder.

(b) Lane 1, 1kb DNA ladder; Lane 2, λ DNA alone (0.5 μg); Lane 3, λ DNA + 50 μM **2**; Lane 4, λ DNA + 5 unit Ssp I (control); Lane 5, λ DNA + 5 unit Ssp I + 50 μM **3**; Lane 6, λ DNA + 5 unit Ase I (control); Lane 7, λ DNA + 5 unit Ase I + 50 μM **3**; Lane 8, λ DNA + 5 unit Mun I (control); Lane 9, λ DNA + 5 unit Mun I + 50 μM **2**; Lane 10, λ DNA + 5 unit EcoR I (control); Lane 11, λ DNA + 5 unit EcoR I + 50 μM **2**; Lane 12, λ DNA + 5 unit NdeI (control); Lane 13, λ DNA + 5 unit NdeI + 50 μM **2**; Lane 14, λ DNA + 5 unit Bst 11071 (control); Lane 15, λ DNA + 5 unit Bst 11071 + 50 μM **2**; Lane 16, 1kb DNA ladder.

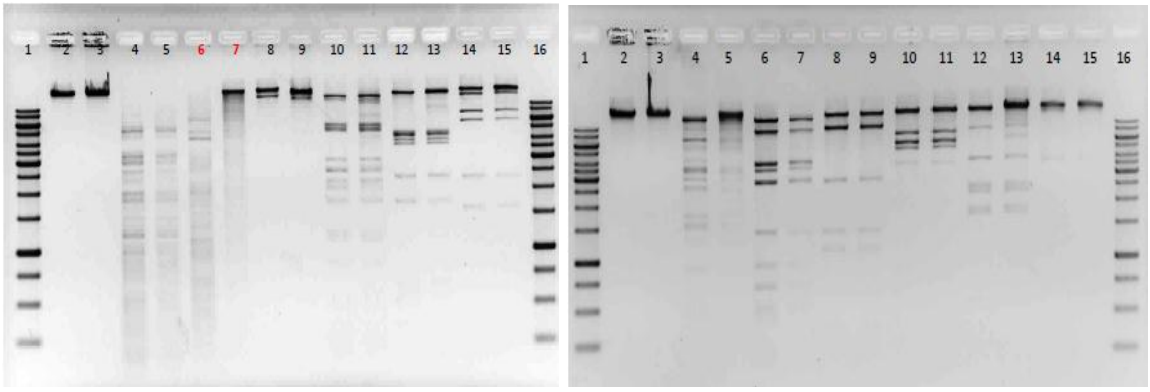


Figure S3.5 RE inhibition by **3**.

Electrophoresis results of incubating λ DNA (0.5 μg/μL) with 5 unit of restriction enzyme in the presence or absence of 50 μM **3** for 2 hours at 37ºC.

(a) Lane 1, 1kb DNA ladder; Lane 2, λ DNA alone (0.5 μg); Lane 3, λ DNA + 50 μM **3**; Lane 4, λ DNA + 5 unit Tsp 509I (control); Lane 5, λ DNA + 5 unit Tsp 509I + 50 μM **3**; Lane 6, λ DNA + 5 unit Hae III (control); Lane 7, λ DNA + 5 unit Hae III + 50 μM **3**; Lane 8, λ DNA + 5 unit Sal I (control); Lane 9, λ DNA + 5 unit Sal I + 50 μM **3**; Lane 10, λ DNA + 5 unit Pst I (control); Lane 11, λ DNA + 5 unit Pst I + 50 μM **3**; Lane 12, λ DNA + 5 unit Pvu II (control); Lane 13, λ DNA + 5 unit Pvu II + 50 μM **3**; Lane 14, λ DNA + 5 unit Sca I (control); Lane 15, λ DNA + 5 unit Sca I + 50 μM **3**; Lane 16, 1kb DNA ladder.

(b) Lane 1, 1kb DNA ladder; Lane 2, λ DNA alone (0.5 μg); Lane 3, λ DNA + 50 μM **3**; Lane 4, λ DNA + 5 unit Ssp I (control); Lane 5, λ DNA + 5 unit Ssp I + 50 μM **3**; Lane 6, λ DNA + 5 unit Ase I (control); Lane 7, λ DNA + 5 unit Ase I + 50 μM **3**; Lane 8, λ DNA + 5 unit Mun I (control); Lane 9, λ DNA + 5 unit Mun I + 50 μM **3**; Lane 10, λ DNA + 5 unit EcoR I (control); Lane 11, λ DNA + 5 unit EcoR I + 50 μM **3**; Lane 12, λ DNA + 5 unit NdeI (control); Lane 13, λ DNA + 5 unit NdeI + 50 μM **3**; Lane 14, λ DNA + 5 unit Bst 11071 (control); Lane 15, λ DNA + 5 unit Bst 11071 + 50 μM **3**; Lane 16, 1kb DNA ladder.

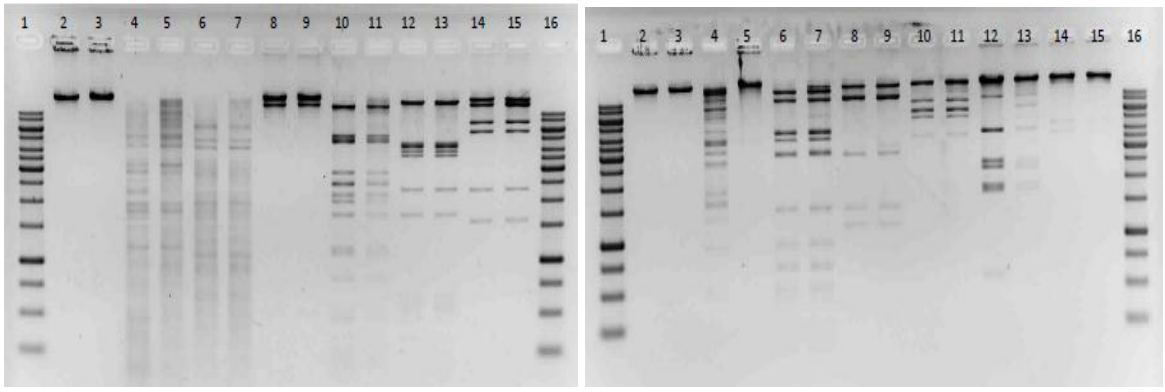


Figure S3.6 RE inhibition by **4**.

Electrophoresis results of incubating λ DNA (0.5 μg/μL) with 5 unit of restriction enzyme in the presence or absence of 50 μM **4** for 2 hours at 37ºC.

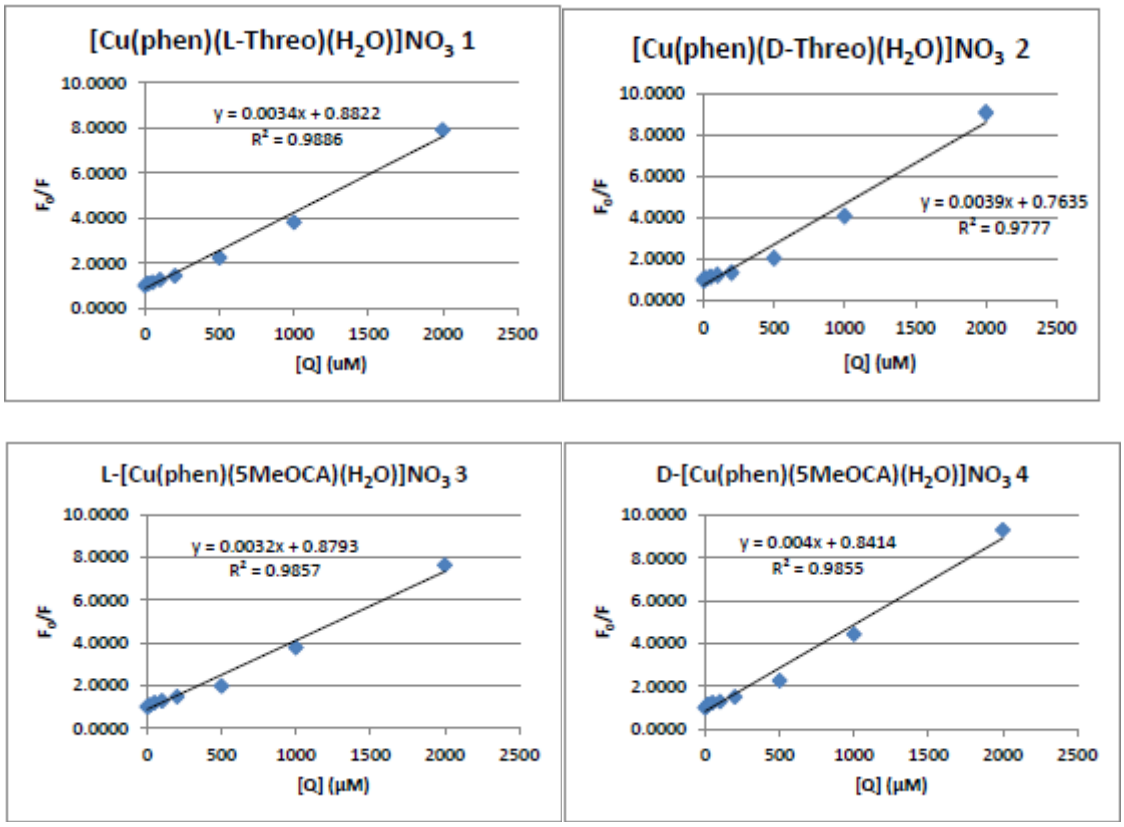
(a) Lane 1, 1kb DNA ladder; Lane 2, λ DNA alone (0.5 μg); Lane 3, λ DNA + 50 μM **4**; Lane 4, λ DNA + 5 unit Tsp 509I (control); Lane 5, λ DNA + 5 unit Tsp 509I + 50 μM **4**; Lane 6, λ DNA + 5 unit Hae III (control); Lane 7, λ DNA + 5 unit Hae III + 50 μM **4**; Lane 8, λ DNA + 5 unit Sal I (control); Lane 9, λ DNA + 5 unit Sal I + 50 μM **4**; Lane 10, λ DNA + 5 unit Pst I (control); Lane 11, λ DNA + 5 unit Pst I + 50 μM **4**; Lane 12, λ DNA + 5 unit Pvu II (control); Lane 13, λ DNA + 5 unit Pvu II + 50 μM **4**; Lane 14, λ DNA + 5 unit Sca I (control); Lane 15, λ DNA + 5 unit Sca I + 50 μM **4**; Lane 16, 1kb DNA ladder.

(b) Lane 1, 1kb DNA ladder; Lane 2, λ DNA alone (0.5 μg); Lane 3, λ DNA + 50 μM **4**; Lane 4, λ DNA + 5 unit Ssp I (control); Lane 5, λ DNA + 5 unit Ssp I + 50 μM **4**; Lane 6, λ DNA + 5 unit Ase I (control); Lane 7, λ DNA + 5 unit Ase I + 50 μM **4**; Lane 8, λ DNA + 5 unit Mun I (control); Lane 9, λ DNA + 5 unit Mun I + 50 μM **4**; Lane 10, λ DNA + 5 unit EcoR I (control); Lane 11, λ DNA + 5 unit EcoR I + 50 μM **4**; Lane 12, λ DNA + 5 unit NdeI (control); Lane 13, λ DNA + 5 unit NdeI + 50 μM **4**; Lane 14, λ DNA + 5 unit Bst 11071 (control); Lane 15, λ DNA + 5 unit Bst 11071 + 50 μM **4**; Lane 16, 1kb DNA ladder.

(C) FL spectra of BSA in the absence and presence of **1**-**4** (Figs. S4.1-S4.4 (a), (b), (c))

The experiment to obtain the FL emission spectra of BSA in the absence and presence of increasing concentration of **1**-**4** [0 (a), 2 (b), 4 (c), 10 (d), 20 (e), 40 (f), 100 (g), 200 (h) and 400 (i) μM] were done in triplicate. See **Appendix II**.

(D) Stern-Volmer plots of Fo/F vs [Q] for **1**-**4** (Figs. S5.1-S5.4)



Figs. S5.1-S5.4 Stern-Volmer plots of Fo/F vs [Q] for **1**-**4**

(E) Plots of log(ΔF/F) vs log[Q] for **1-4** (Figs. S6.1-S6.4)

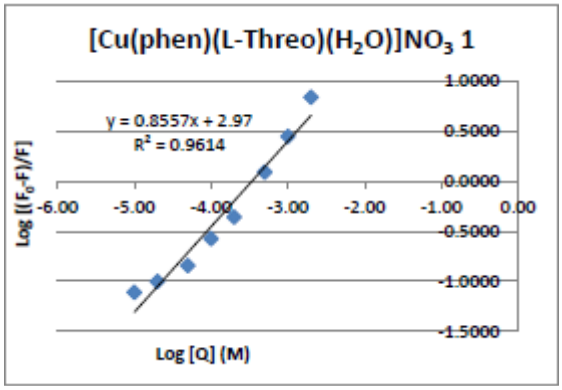


Fig. S6.1

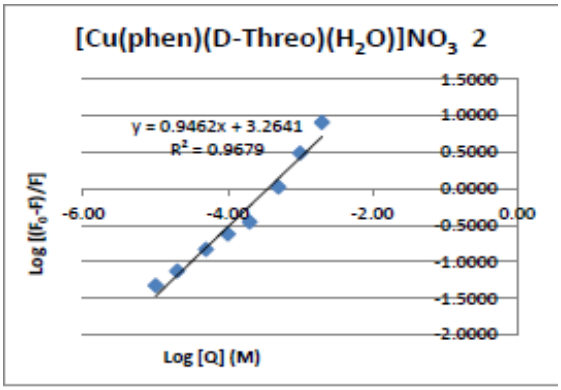
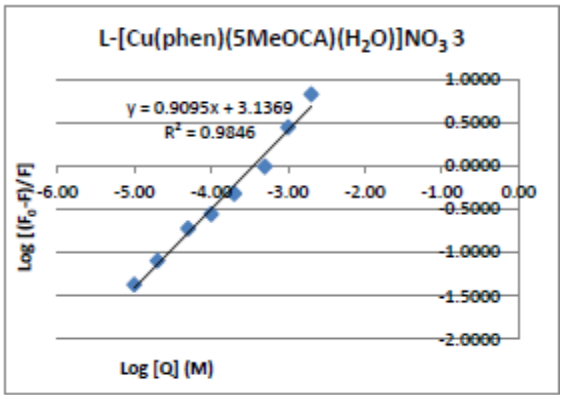


Fig. S6.2



Figs. S6.3

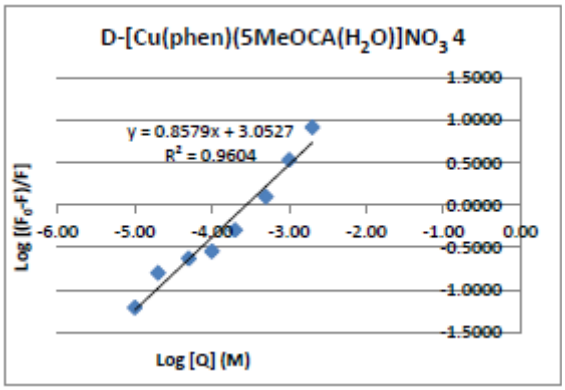


Fig. S6.4

Figs. S6.1-S6.4 Plots of log(ΔF/F) vs log[Q] for **1-4**.

(F) UV spectra of BSA in absence and presence of increasing concentration of **1**-**4** (Figs. S671-S7.4)

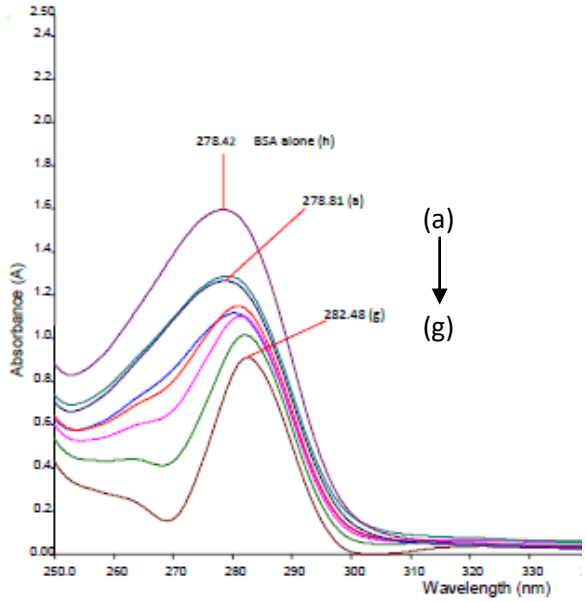


Fig. S7.1 for **1**

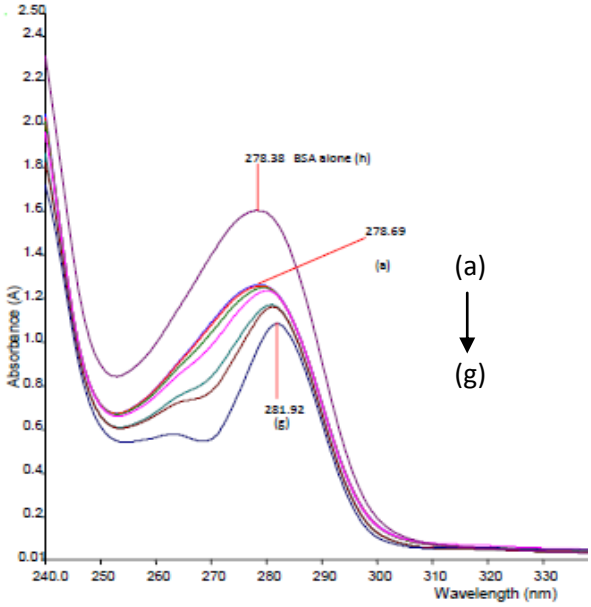


Fig. S7.2 for **2**

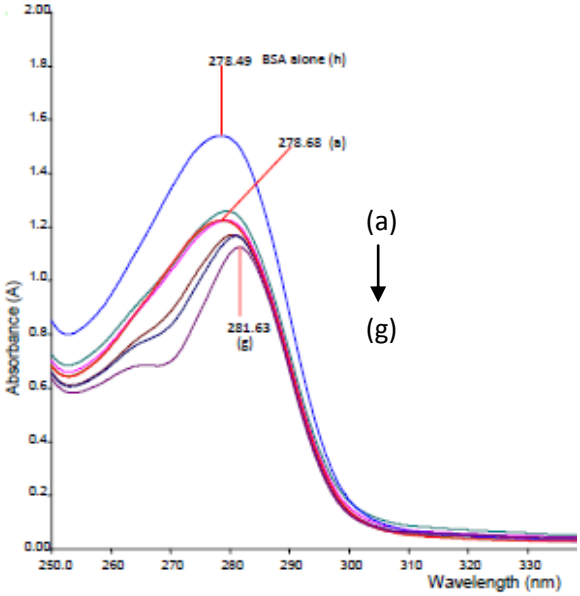


Fig. S7.3 for **3**

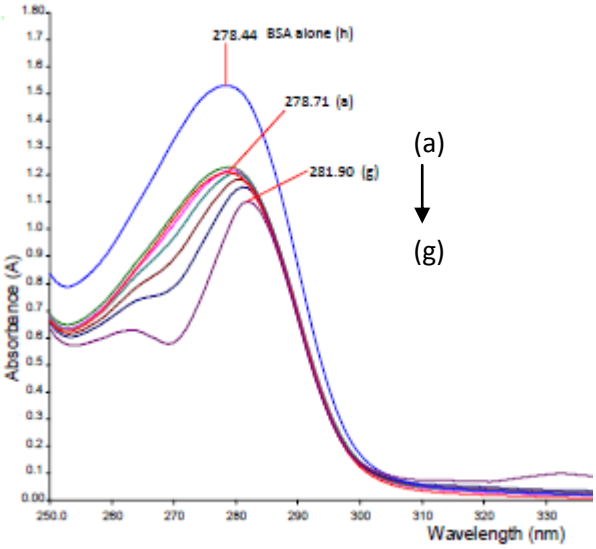


Fig. S7.4 for **4**

Figures S7.1-S7.4. Absorption spectra of BSA in the absence (h) and presence of increasing concentration [2 (a), 4 (b), 10 (c), 20 (d), 30 (e), 40 (f) and 50 μM (g)] of copper(II) complexes (1-4). Concentration of BSA alone in the absence of complex was 32.5 μM (h).

(G) Synchronous FL spectra of BSA in the absence (*a*) and presence of increasing concentration [2 (*b*), 4 (*c*), 10 (*d*), 20 (*e*), 40 (*f*), 100 (*g*), 200 (*h*) and 400 (*i*) μM] of **1**-**4** at (a) $\Delta\lambda$ = 15 nm (tyrosine); (b) $\Delta\lambda$ = 60 nm (tryptophan) (Figs. S8.1-S8.4 (a) and (b))

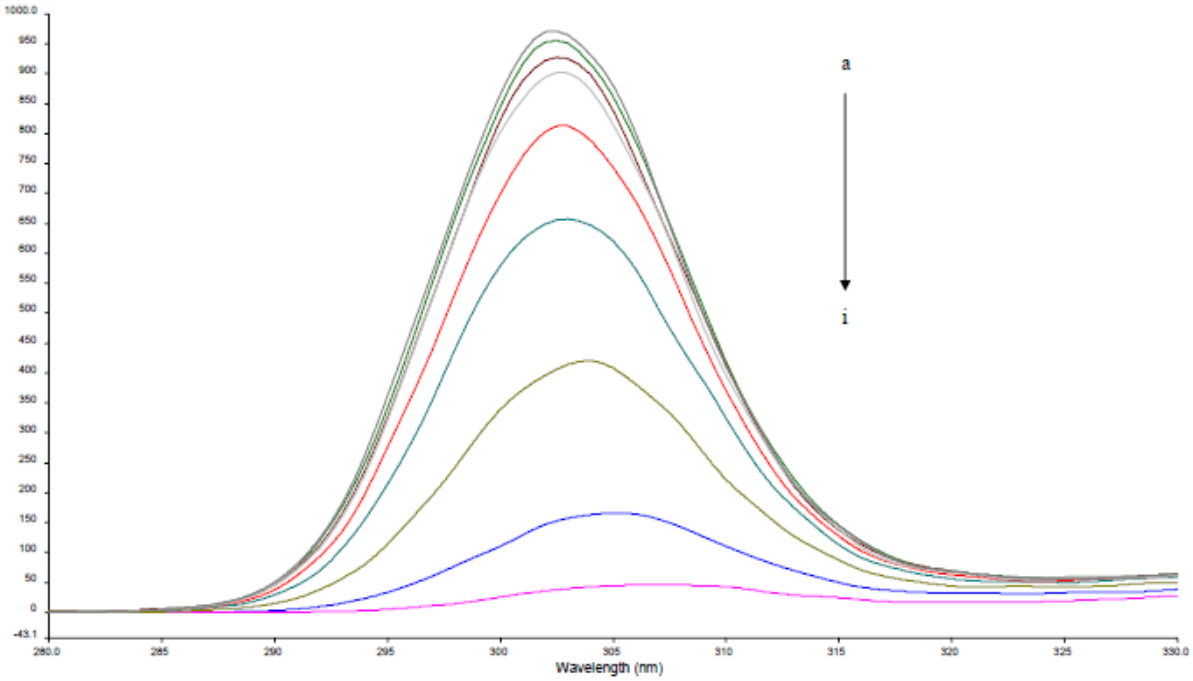


Fig. S8.1(a) for **1**

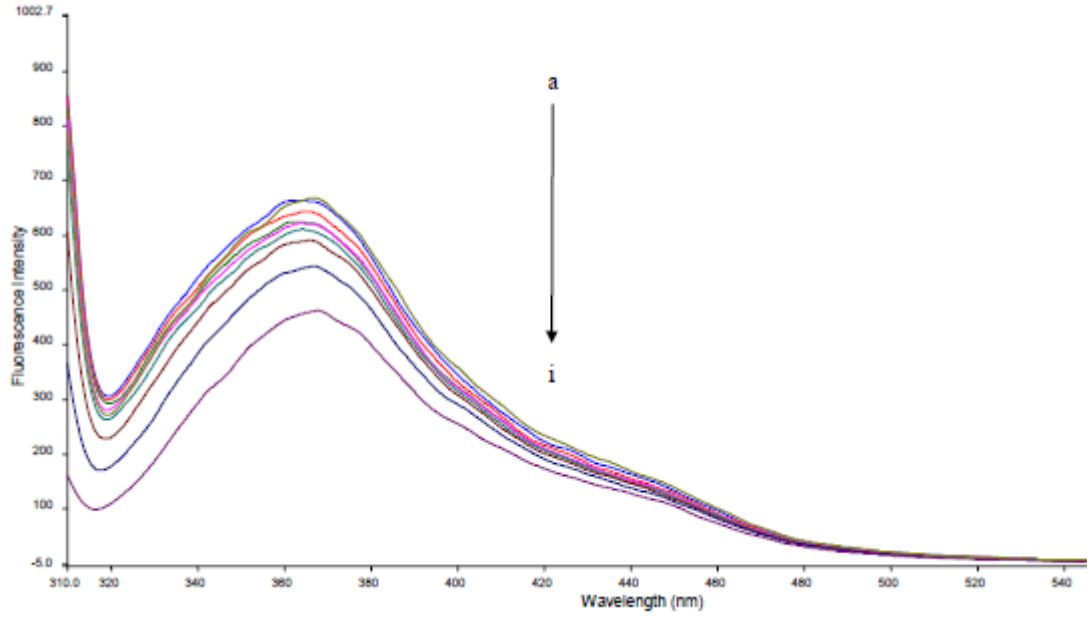


Fig. S8.1(b) for **1**

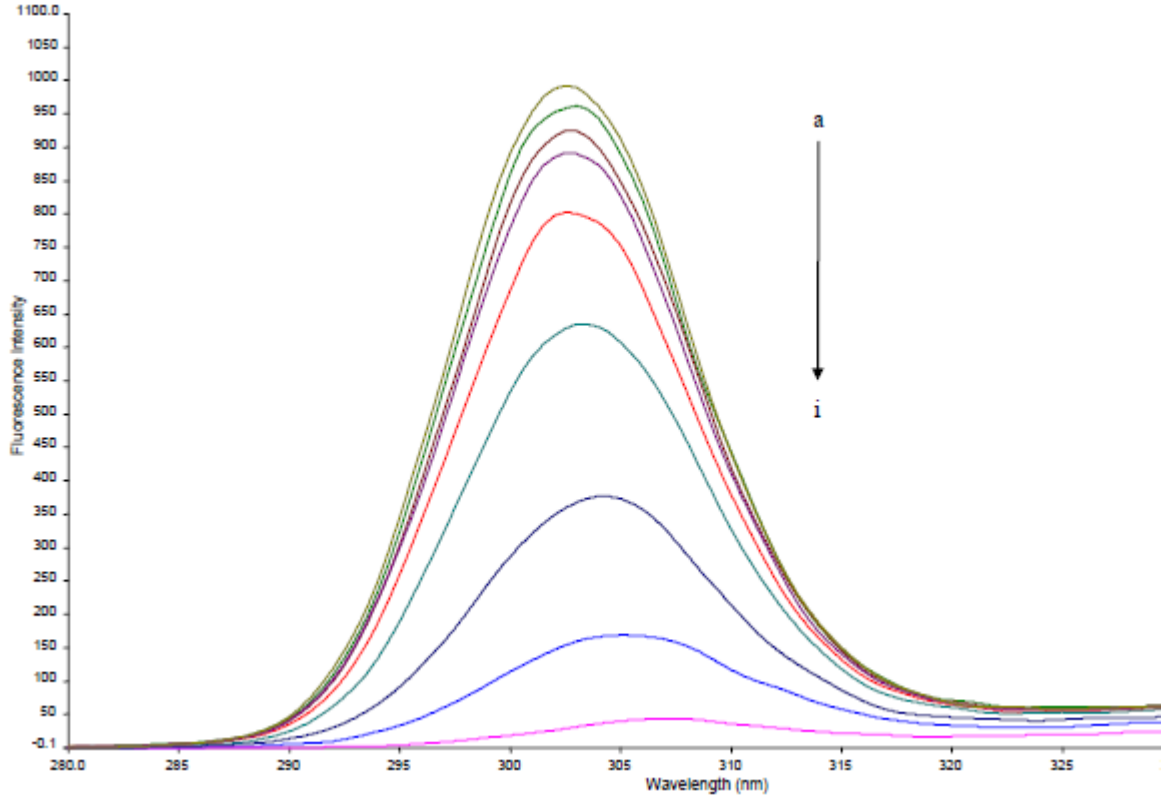


Fig. 8.2(a) for **2**

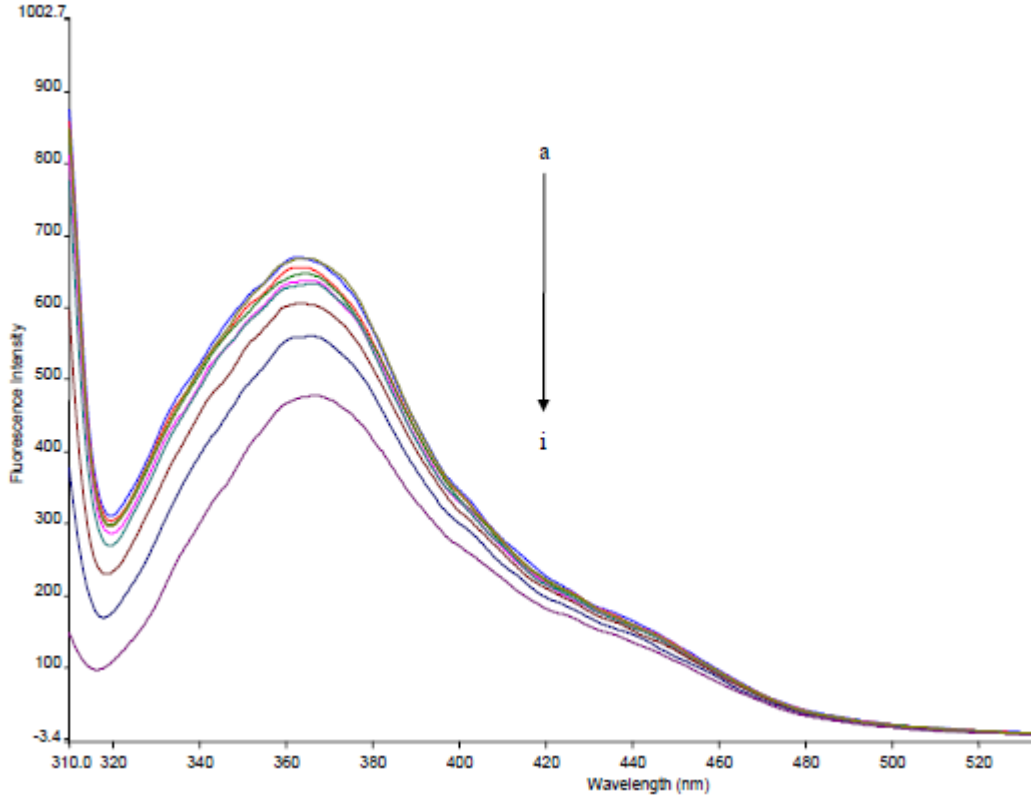


Fig. 8.2(b) for **2**

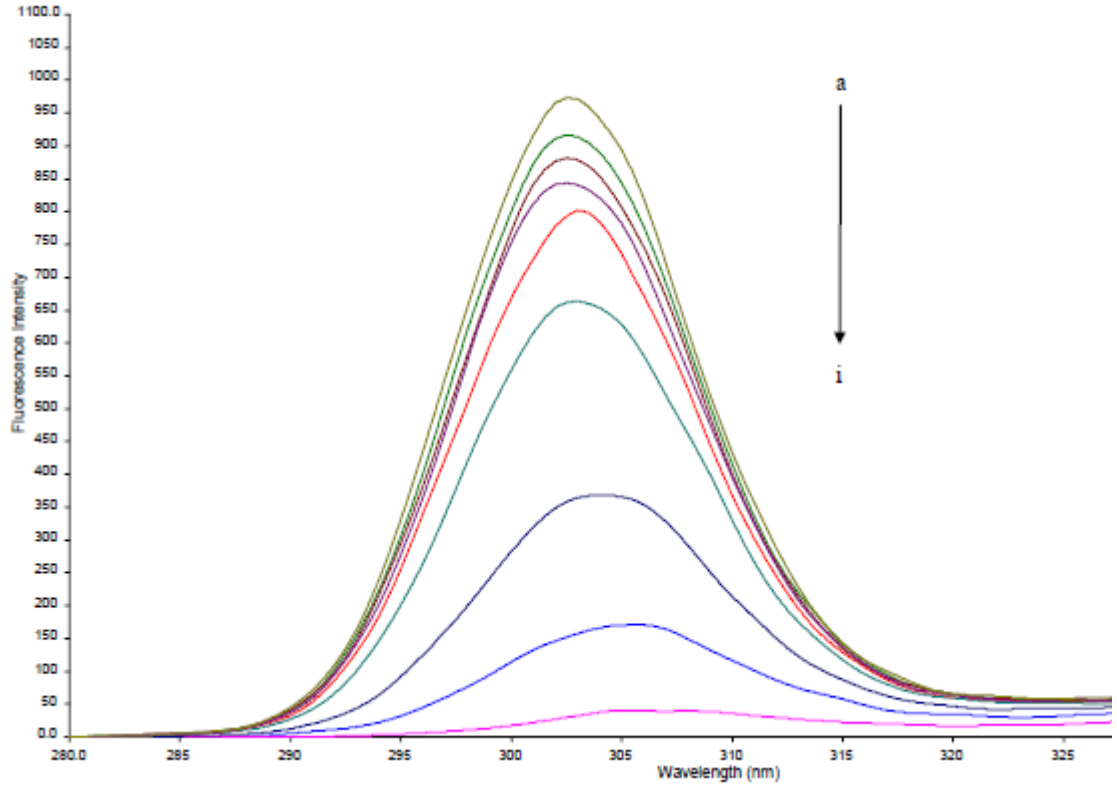


Fig. 8.3(a) for **3**

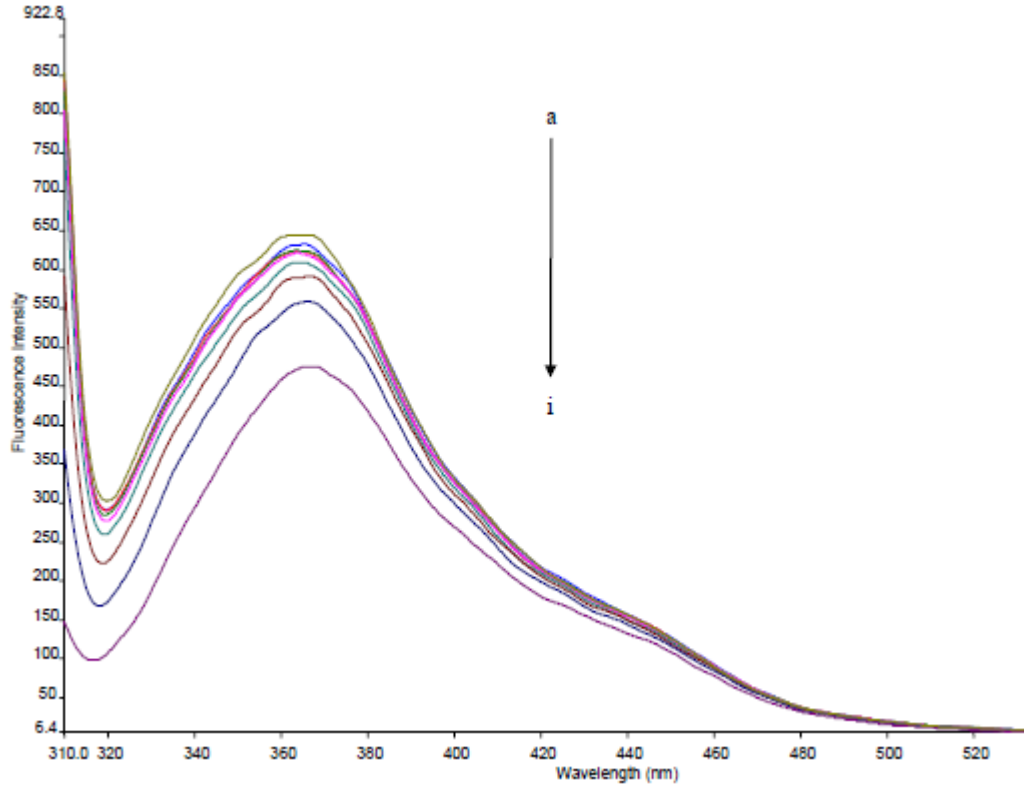


Fig. 8.3(b) for **3**

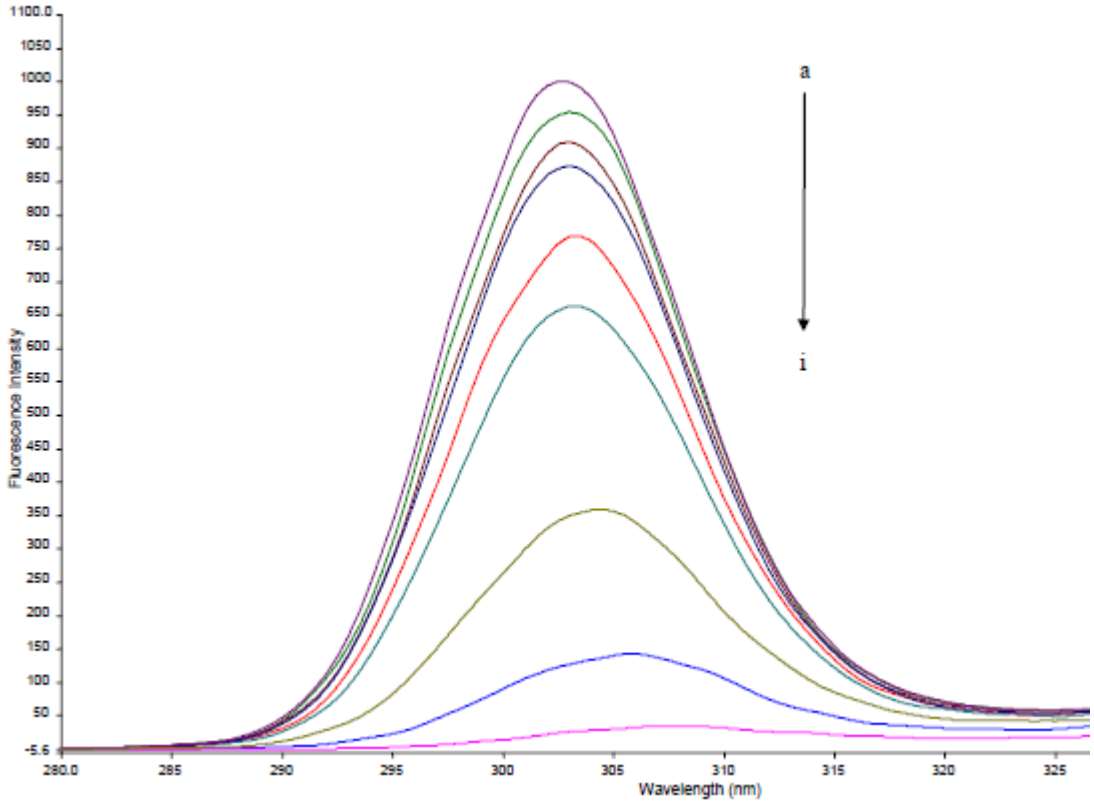


Fig. S8.4(a) for **4**

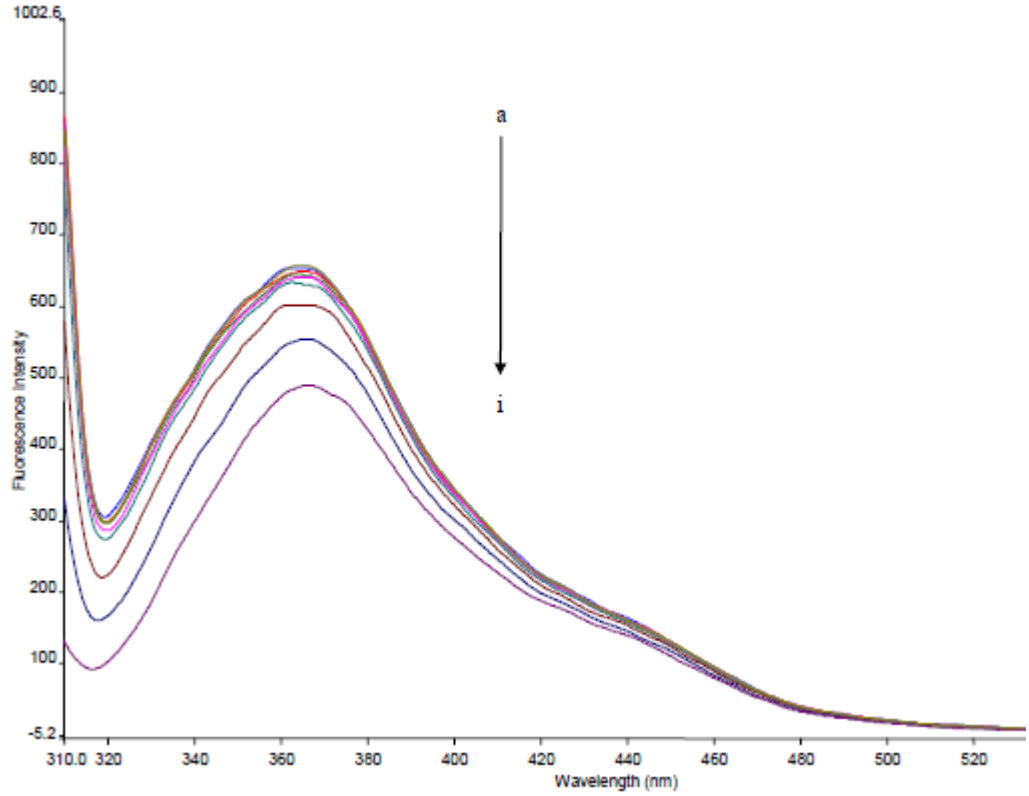


Fig. S8.4(b) for **4**

Figs. S8.1-S8.4 Synchronous FL spectra of BSA in the absence (*a*) and presence of increasing concentration of **1**-**4** [2 (*b*), 4 (*c*), 10 (*d*), 20 (*e*), 40 (*f*), 100 (*g*), 200 (*h*) and 400 (*i*) μM] at (a) Δλ = 15 nm (tyrosine); (b) Δλ = 60 nm (tryptophan)

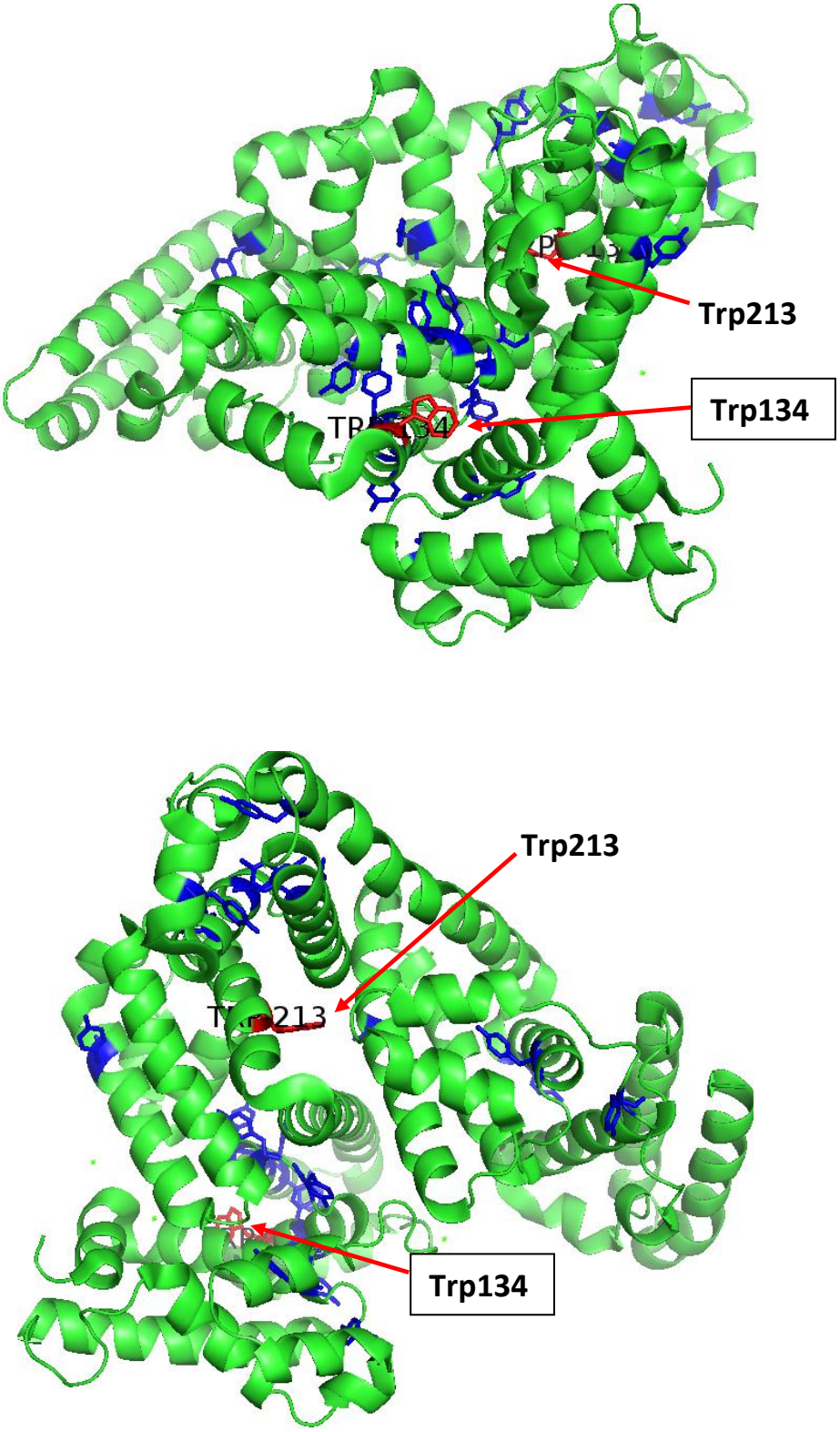


Fig. S9 Comparison of Trp134 and Trp213 binding sites. The **Trp134-binding site** (Top) (Red = Trp134; blue = Tyr residue) has Trp134 with nearby Tyr residues (140, 142, 148, 149, 153). Trp134 is located in the hydrophobic pocket of subdomain IA near the protein surface. **Trp213-binding site** (bottom) containsTrp213 with no nearby Tyr residues but has charged Arg and Asp residues (not shown). Trp213 is in the hydrophobic core of subdomain IIA

Supplementary Tables S1 and S2
Crystallographic data and selected bond lengths and angles of **3** and **4**

Table S1 Crystal data and structure refinement for **3** and **4**

	3	**4**
Empirical formula	$C_{17}H_{19.25}N_4O_{7.63}Cu$	$C_{17}H_{19.25}N_4O_{7.63}Cu$
Formula weight	465.15	465.15
Temperature, K	103(2)	100(2)
Wavelength, Å	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space group	*P1*	*P1*
Unit cell dimensions	a = 7.6300(4) Å α= 81.2860(10)° *b* = 10.8699(7) Å β= 84.1770(10)° *c* = 11.7670(7) Å γ = 75.6260(10)°	*a* = 7.6383(3)Å α = 81.250(2)° *b* = 10.8787(4)Å β= 84.085(2) ° *c* = 11.7750(4) Å γ =75.541(2) °
Volume, $Å^3$	932.38(10)	934.26(6)
Z	2	2
Density (calculated), mg/m^3	1.657	1.654
Absorption coefficient, mm^{-1}	1.226	1.223
F(000)	479	479
Crystal size, mm^3	0.40 x 0.20 x 0.20	0.40 x 0.38 x 0.20
θ range for data collection	2.45 to 30.56°	2.45 to 26.37°
Index ranges	$-7 \le h \le 9$, $-13 \le k \le 13$, $-14 \le l \le 14$	$-9 \le h \le 9$, $-13 \le k \le 13$, $-14 \le l \le 14$
Reflections collected	11702	25521
Independent reflections	5712 [*R*(int) = 0.0456]	6572[*R*(int) = 0.0440]
Absorption correction	Multi-scan	Multi-scan
Max. and min. transmission	0.7916 and 0.6399	0.7920 and 0.6404
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	5984 / 3 / 549	6972 / 17 / 557
Goodness-of-fit on F_2	1.043	1.074
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0272, wR_2 = 0.0703	R_1 = 0.0367, wR_2 = 0.0938
R indices (all data)	R_1 = 0.0290, wR_2 = 0.0714	R_1 = 0.0337, wR_2 = 0.0873
Largest diff. peak and hole, e $Å^{-3}$	0.771 and -0.586	0.717 and -0.689

Tables S2.1 and S2.2 Selected bond lengths and angles for **3** and **4**.

Table S2.1 Selected bond lengths (Å) and angles (°) for **3**

Bond lengths (Å)			
C(1) – O(2)	1.222 (5)	C(5) – O(3)	1.414 (4)
C(1) – O(1)	1.270 (4)	C(5) – N(1)	1.473 (4)
C(1) – C(2)	1.529 (4)	Cu(1) – O(1)	1.932 (3)
C(2) – N(1)	1.485 (4)	Cu(1) – N(3)	1.992 (4)
C(2) – C(3)	1.546 (4)	Cu(1) – N(1)	2.002 (3)
C(3) – O(3)	1.422 (4)	Cu(1) – N(2)	2.013 (3)
C(3) – C(4)	1.503 (5)	Cu(1) – O(4)	2.285 (3)
Bond angles (°)			
O(2) – C(1) – O(1)	124.5 (3)	O(1) – Cu(1) – N(3)	92.34 (13)
O(2) – C(1) – C(2)	118.3 (3)	O(1) – Cu(1) – N(1)	85.15 (12)
O(1) – C(1) – C(2)	117.1 (3)	N(3) – Cu(1) – N(1)	177.15 (15)
N(1) – C(2) – C(1)	111.2 (3)	O(1) – Cu(1) – N(2)	169.35 (13)
N(1) – C(2) – C(3)	104.6 (3)	N(3) – Cu(1) – N(2)	82.67 (14)
C(1) – C(2) – C(3)	112.1 (3)	N(1) – Cu(1) – N(2)	99.59 (13)
O(3) – C(3) – C(4)	109.4 (3)	O(1) – Cu(1) – O(4)	88.69 (10)
O(3) – C(3) – C(2)	104.0 (2)	N(3) – Cu(1) – O(4)	95.12 (12)
C(4) – C(3) – C(2)	114.7 (3)	N(1) – Cu(1) – O(4)	86.18 (11)
O(3) – C(5) – N(1)	104.9 (3)	N(2) – Cu(1) – O(4)	101.08 (11)
C(5) – N(1) – C(2)	104.2 (3)	C(5) – O(3) – C(3)	105.3 (2)
C(5) – N(1) – Cu(1)	120.7 (2)	C(1) – O(1) – Cu(1)	114.9 (2)
C(2) – N(1) – Cu(1)	106.9 (2)		

Table S2.2: Selected bond lengths (Å) and angles (°) for **4**

Bond lengths (Å)			
C(1A) – O(2A)	1.229 (5)	C(5A) – O(3A)	1.415 (4)
C(1A) – O(1A)	1.272 (5)	C(5A) – N(1A)	1.470 (5)
C(1A) – C(2A)	1.532 (5)	Cu(1A) – O(1A)	1.932 (3)
C(2A) – N(1A)	1.484 (5)	Cu(1A) – N(3A)	1.990 (4)
C(2A) – C(3A)	1.545 (5)	Cu(1A) – N(1A)	2.005 (3)
C(3A) – O(3A)	1.426 (4)	Cu(1A) – N(2A)	2.016 (4)
C(3A) – C(4A)	1.503 (5)	Cu(1A) – O(4A)	2.290 (3)
Bond angles (°)			
O(2A) – C(1A) – O(1A)	124.3 (4)	O(1A) – Cu(1A) – N(3A)	92.36 (14)
O(2A) – C(1A) – C(2A)	118.2 (3)	O(1A) – Cu(1A) – N(1A)	84.97 (14)
O(1A) – C(1A) – C(2A)	117.4 (3)	N(3A) – Cu(1A) – N(1A)	177.04 (17)
N(1A) – C(2A) – C(1A)	110.6 (3)	O(1A) – Cu(1A) – N(2A)	169.38 (14)
N(1A) – C(2A) – C(3A)	104.5 (3)	N(3A) – Cu(1A) – N(2A)	82.66 (15)
C(1A) – C(2A) – C(3A)	111.7 (3)	N(1A) – Cu(1A) – N(2A)	99.75 (14)
O(3A) – C(3A) – C(4A)	109.6 (3)	O(1A) – Cu(1A) – O(4A)	88.64 (11)
O(3A) – C(3A) – C(2A)	104.2 (3)	N(3A) – Cu(1A) – O(4A)	94.96 (12)
C(4A) – C(3A) – C(2A)	114.7 (3)	N(1A) – Cu(1A) – O(4A)	86.29 (12)
O(3A) – C(5A) – N(1A)	105.2 (3)	N(2A) – Cu(1A) – O(4A)	101.10 (12)
C(5A) – N(1A) – C(2A)	104.4 (3)	C(5A) – O(3A) – C(3A)	105.1 (2)
C(5A) – N(1A) – Cu(1A)	120.6 (3)	C(1A) – O(1A) – Cu(1A)	114.9 (3)
C(2A) – N(1A) – Cu(1A)	107.3 (2)		

Table S3 UV-visible spectral data of aqueous solutions of phen and **1**-**4** (solvent: water-methanol 1:1 v/v)

Compounds	λ_1/nm (ε/M^{-1} cm^{-1})	λ_2/nm (ε/M^{-1} cm^{-1})	λ_3/nm (ε/M^{-1} cm^{-1})
phen	-	227(40,000)	264(30,000)
1	613 (60)	225 (60,000)	273 (50,000)
2	613 (60)	224 (30,000)	273 (30,000)
3	623 (60)	225 (40,000)	273 (40,000)
4	623 (70)	224 (40,000)	273 (30,000)

Concentration of compounds for visible and UV spectra are $5x10^{-3}$ M and $3x10^{-5}$ M respectively.

Table S4 Molar conductivity (S cm^2 mol^{-1}) for **1**-**4** and other precursor compounds ($1x10^{-3}$ M)

Compounds	0 h	1 h	24 h
1	50	50	50
2	50	50	50
3	50	50	50
4	50	50	50
$Cu(NO_3)_2$	120	120	120
phen	1	1	1
L-threo	1	1	1
D-threo	1	1	1
KCl (standard Solution)	1410	1410	1410

Table S5 Restriction enzymes (REs) inhibited by copper(II) compounds

Compounds	*Hae* III	*Ssp* I	*Ase* I	*Nde* I	*Bst*11071
$CuCl_2$	-	-	-	-	-
$[Cu(phen)Cl_2]$	+	+	+	+	+
1	-	+	-	+	-
2	-	+	-	+	+
3	+	-	-	-	-
4	-	-	+	-	-

RE (binding site): *Hae* III (5'-CGGC-3'); *Ssp* I (5'-AATATT-3'); *Ase* I (5'-ATTAAT-3'); *Nde* I (5'-CATATG-3'); *Bst* 11071 (5'-GTATAC-3')