Electronic Supplementary Information (ESI)

Sensing of tryptophan by a non-toxic Cobalt(II) complex

Swapan Kumar Jana,[a] Amit Kumar Mandal[b], Anoop Kumar[c], Horst Puschmann[d], Maidul Hossain*[a] and Sudipta Dalai*[a]

[a] Department of Chemistry & Chemical Technology, Vidyasagar University, W.B, India. E-mail: sudipta@mail.vidyasagar.ac.in (S.Dalai);
hossainm@mail.vidyasagar.ac.in (M. Hossain)
[b] Department of Microbiology, Vidyasagar University, W.B, India.
[c] Department of Biotechnology, University of North Bengal, W.B, India.
[d] Department of Chemistry, University of Durham, Durham DH13LE, UK.

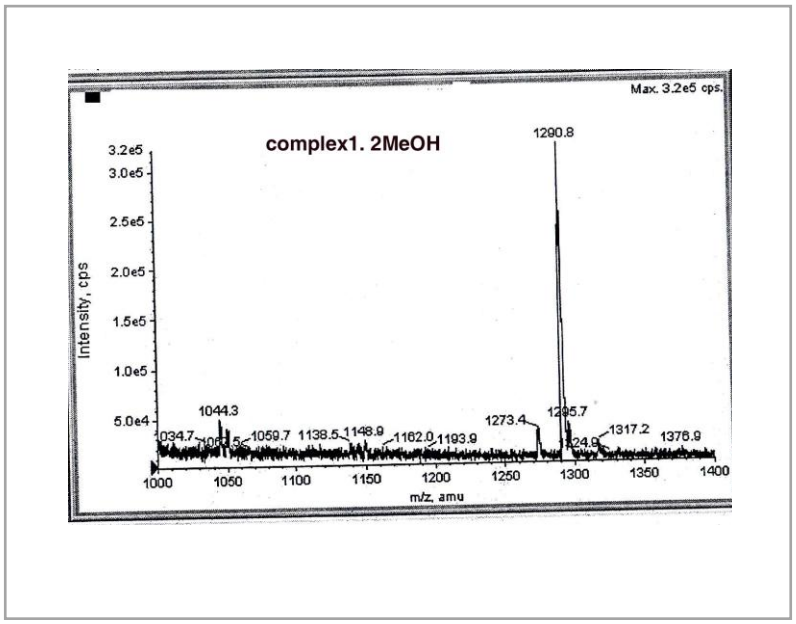

Fig. S1 LC-MS spectrum of complex**1** in MeOH.

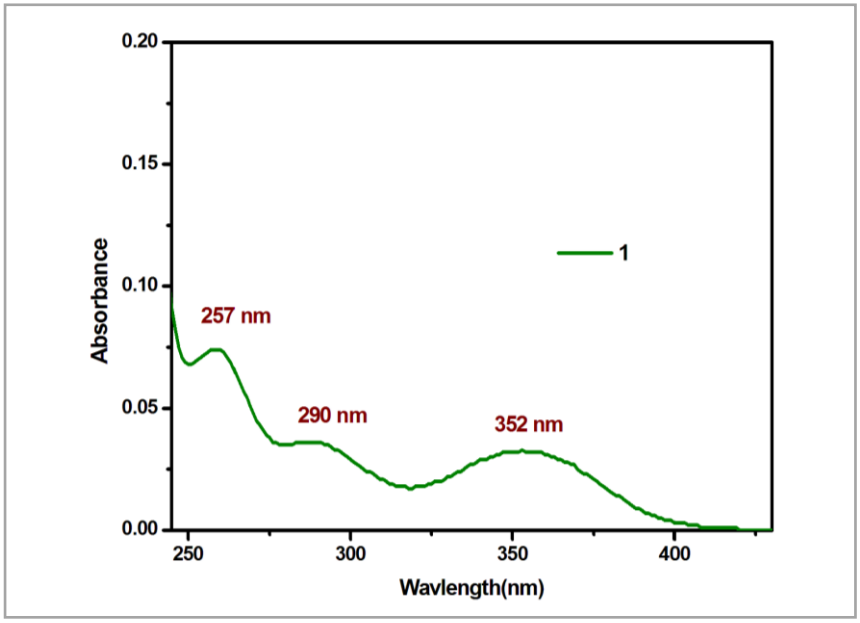

Fig. S2 UV-vis spectra of **1** (1 μM) 1 in PBS buffer (pH = 7.4).

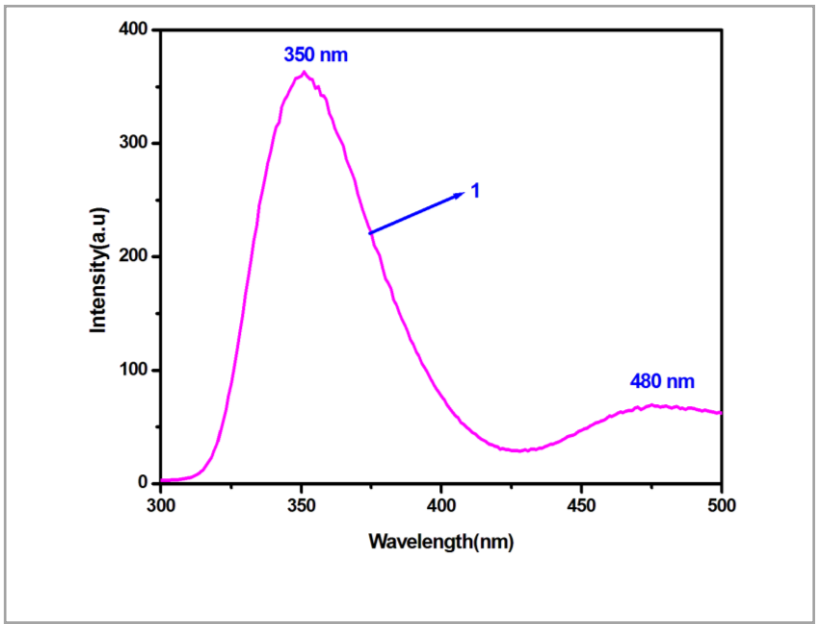

Fig. S3 Fluorescence spectra of **1** (2.5 μM) 1 in PBS buffer (pH = 7.4). (λ_{ex}=257 nm)

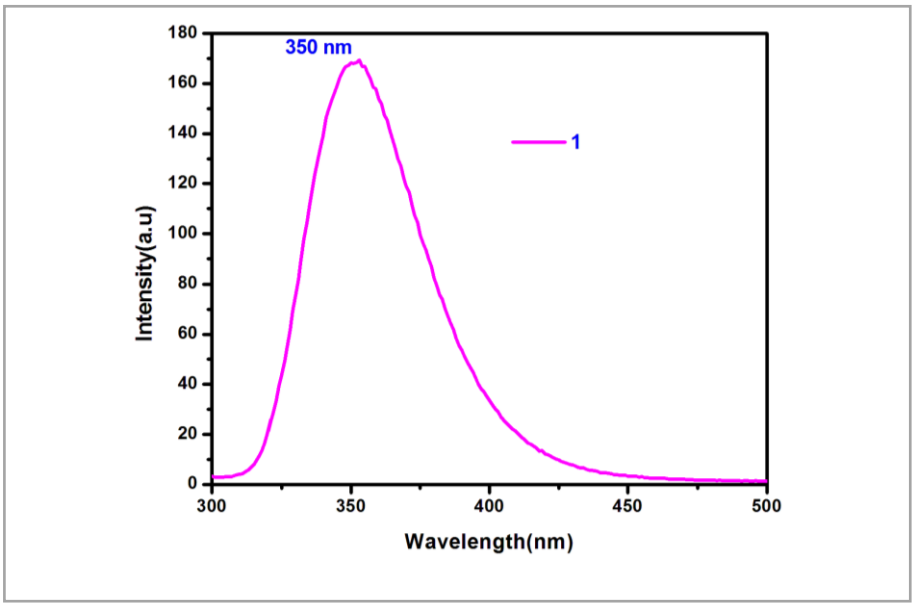

Fig. S4 Fluorescence spectra of **1** (2.5 μM) 1 in PBS buffer (pH = 7.4). (λ_{ex}=290 nm)

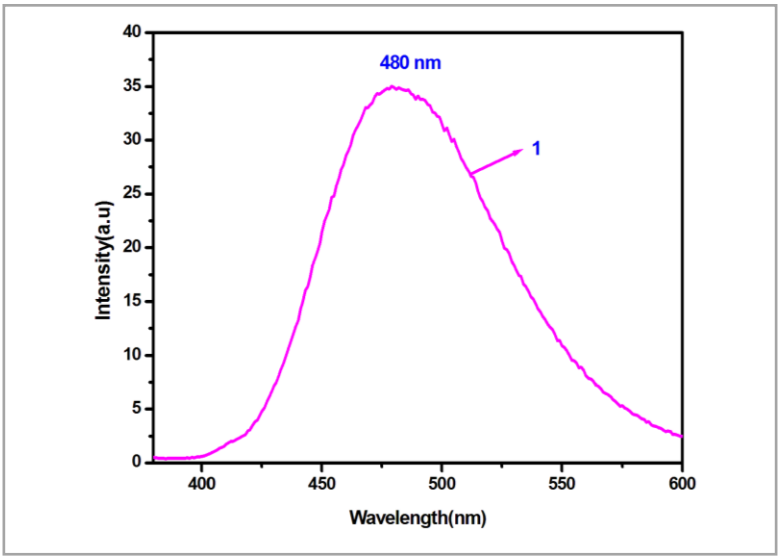

Fig. S5 Fluorescence spectra of **1** (2.5 μM) 1 in PBS buffer (pH = 7.4). (λ_{ex}=352 nm)

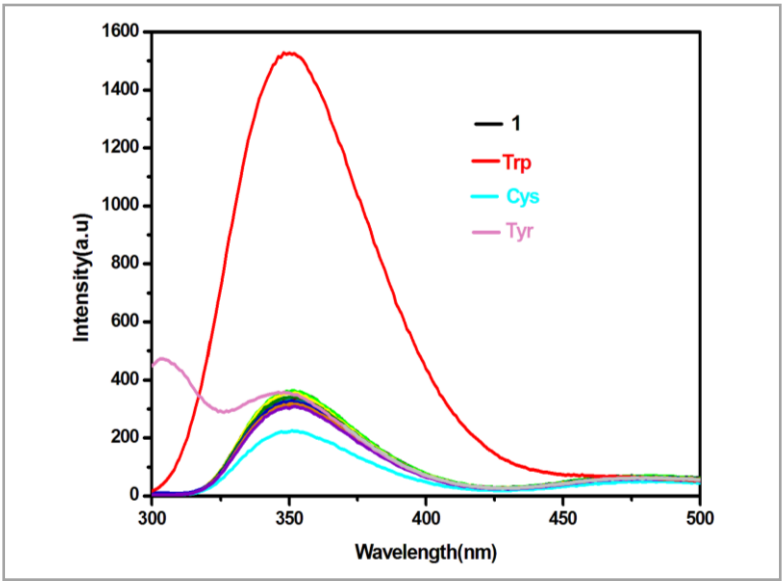

Fig. S6 Fluorescence spectra of **1** (2.5 μM) in the presence of different amino acids (100 μM) in PBS buffer (pH = 7.4). (λ_{ex}=257 nm)

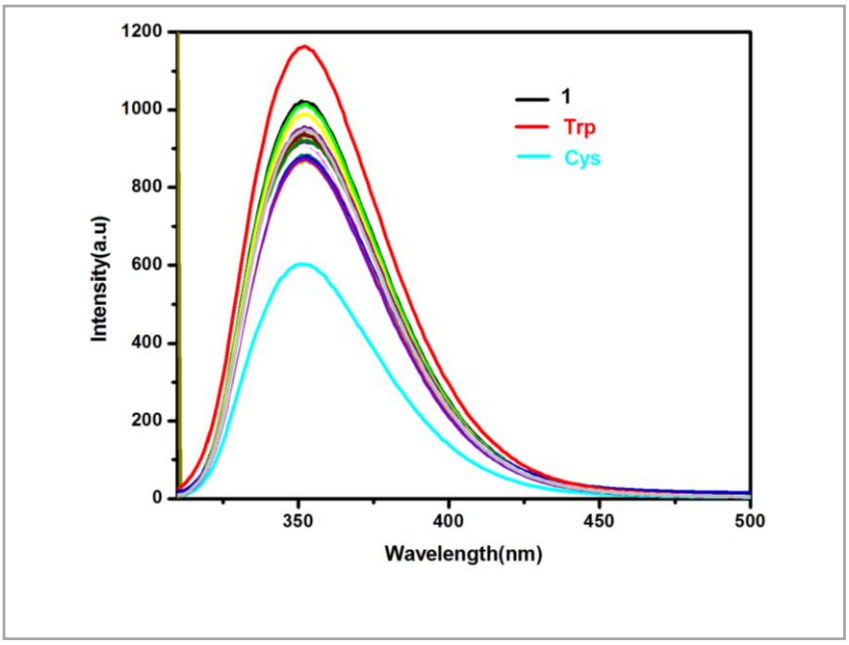

Fig. S7 Fluorescence spectra of **1** (2.5 μM) in the presence of different amino acids (100 μM) in PBS buffer (pH = 7.4). (λ_{ex}=290 nm)

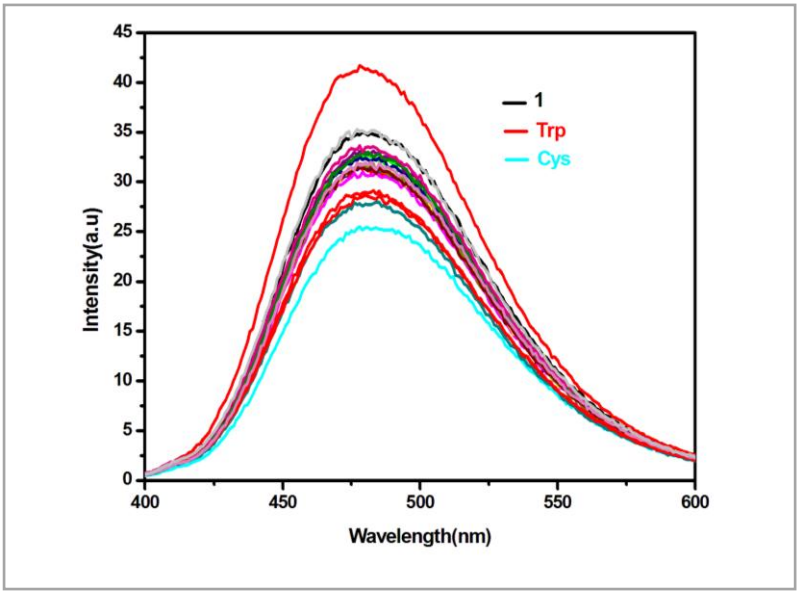

Fig. S8 Fluorescence spectra of **1** (2.5 μM) in the presence of different amino acids (100 μM) in PBS buffer (pH = 7.4). (λ_{ex}=352 nm)

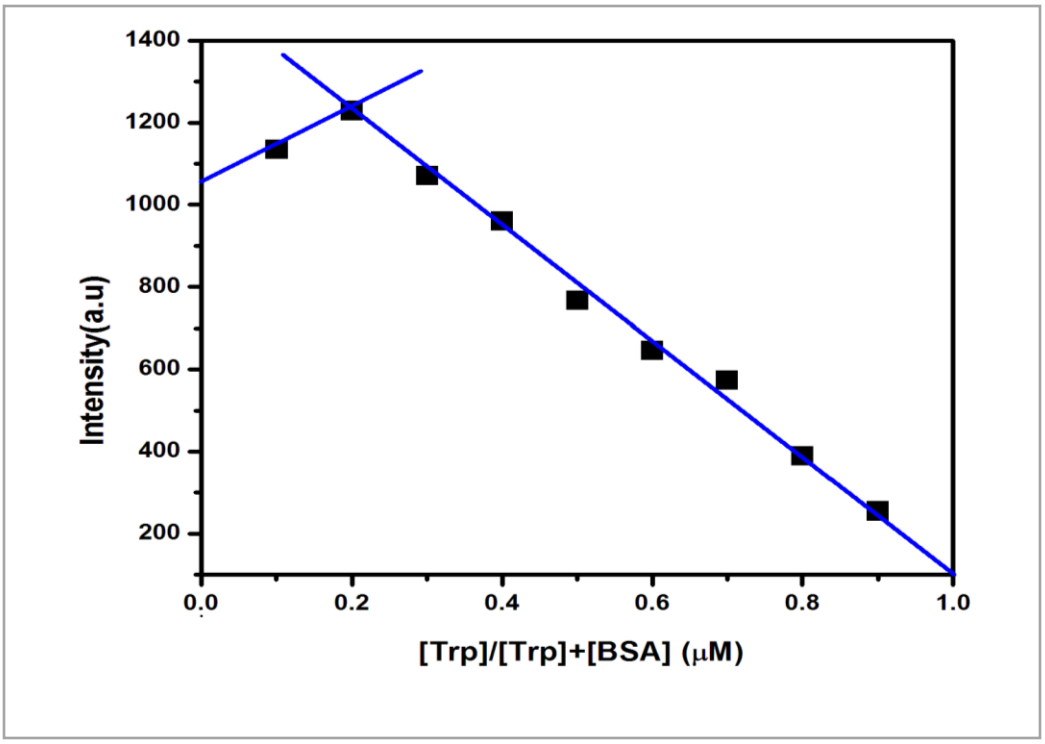

Fig. S9 Job's plot for determining the stoichiometry of **1–Trp** complexation in PBS buffer (pH = 7.4). (λ_{ex}=290 nm)

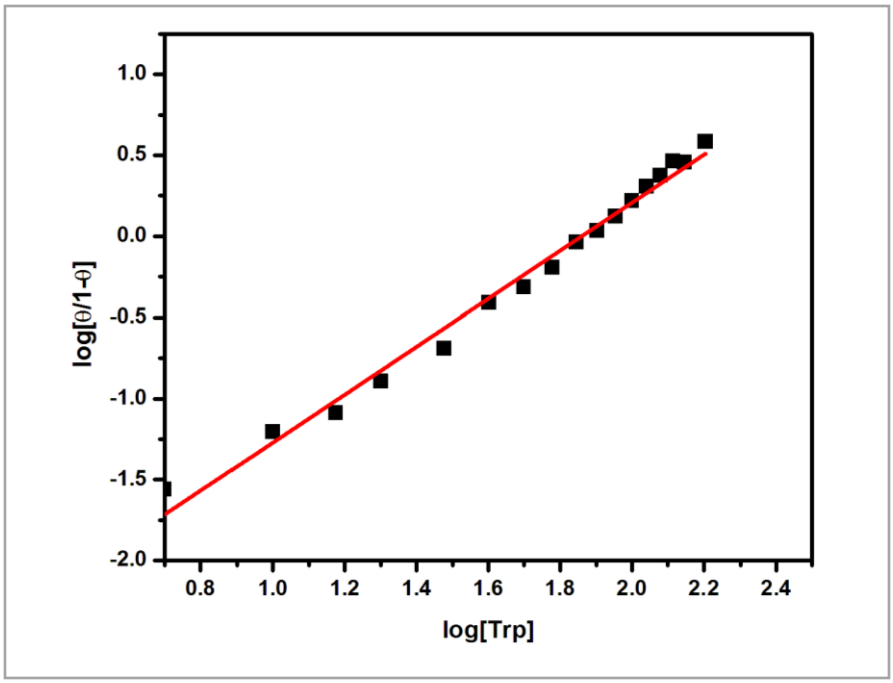

Fig. S10 1-Trp Hill's plot, where legends carry the respective meanings.

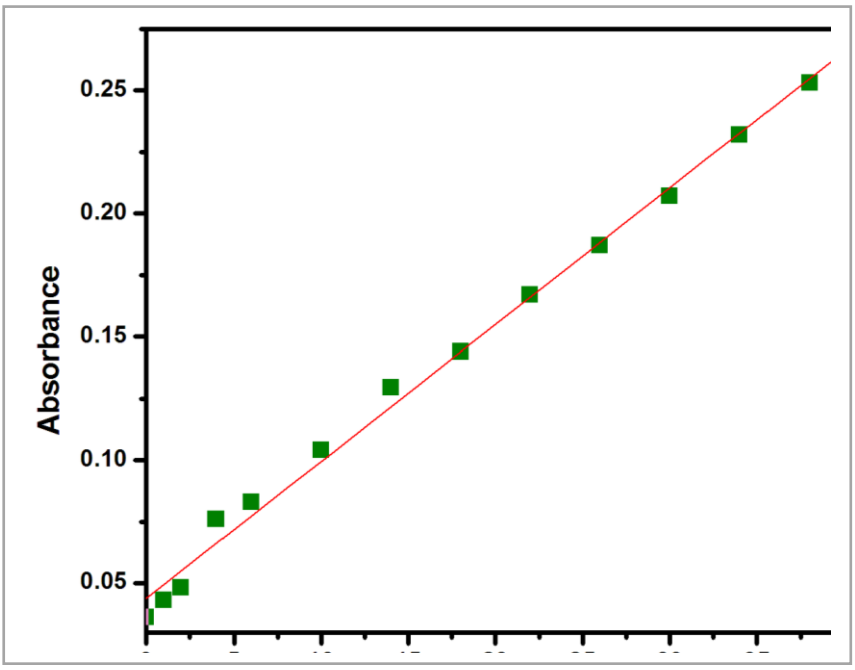

Fig. S11 The absorption of complex**1** (1 μM) at 287 nm as a function of Trp concentration.

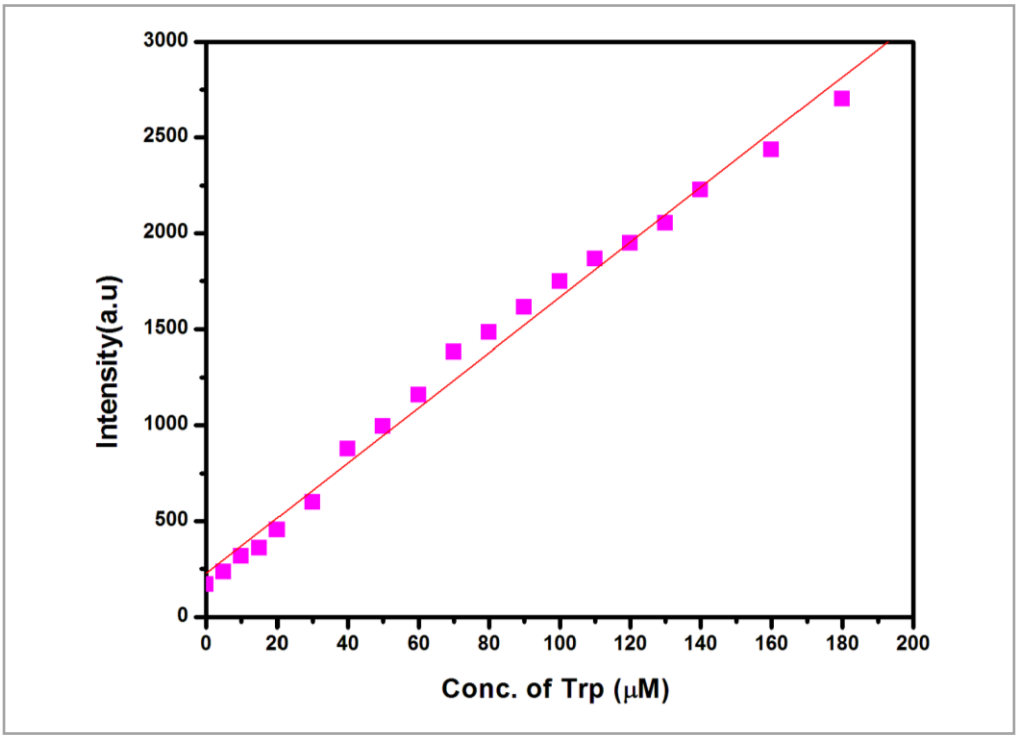

Fig. S12 The fluorescence spectra of complex**1** (0.5 μM) at 350 nm as a function of Trp concentration. (λ_{ex}=290 nm)

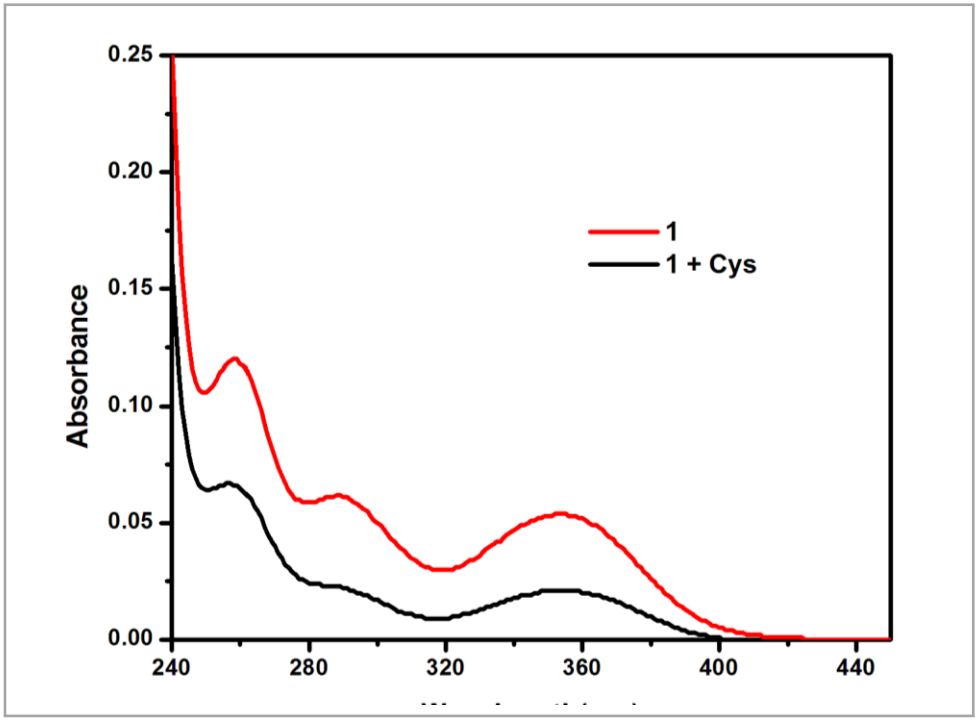

Fig. S13 UV-vis spectra of **1** (1 μM) in both the presence and absence of Cys (40 μM) in PBS buffer (pH = 7.4).

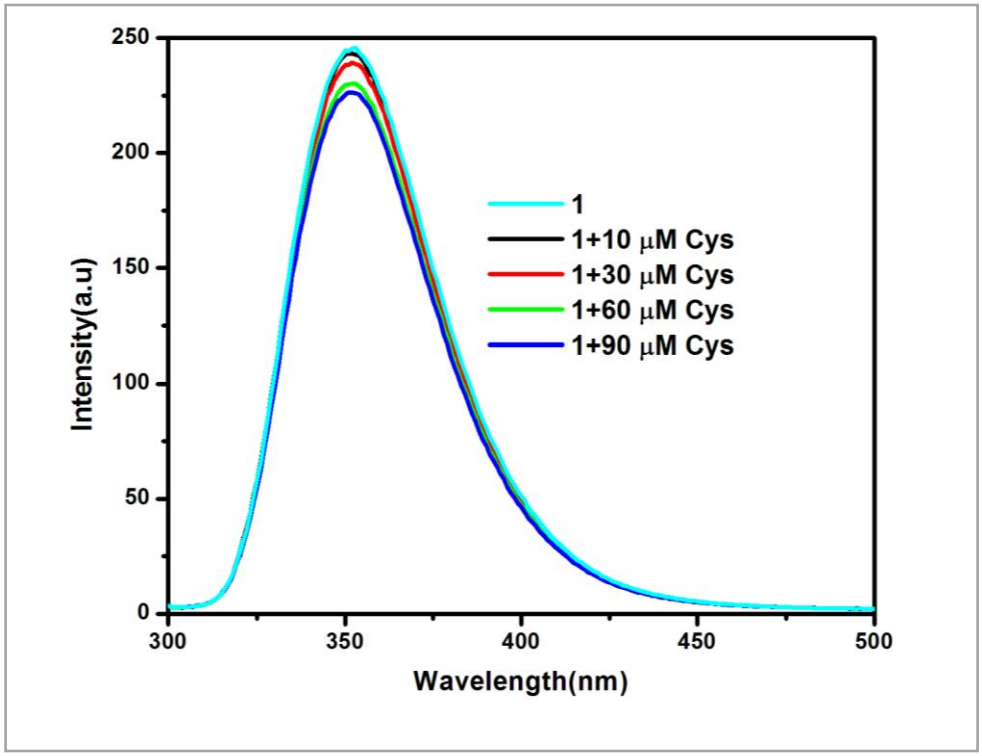

Fig. S14 Fluorescence spectra of **1** (1 μM) in the presence of increasing amount of Cys (0 to 90 μM) in PBS buffer (pH = 7.4). (λ_{ex}=290 nm)

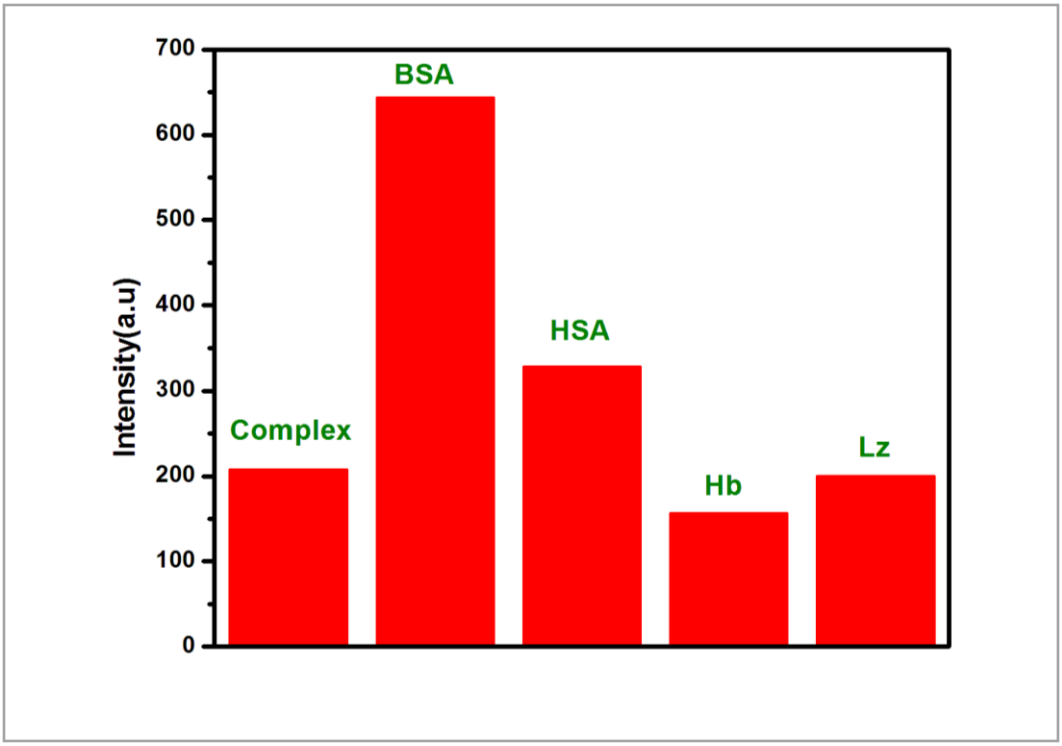

Fig. S15 Bar diagram represents fluorescence spectra of **1** (0.5 μM) in the presence of different proteins (10 μM) in PBS buffer (pH = 7.4).

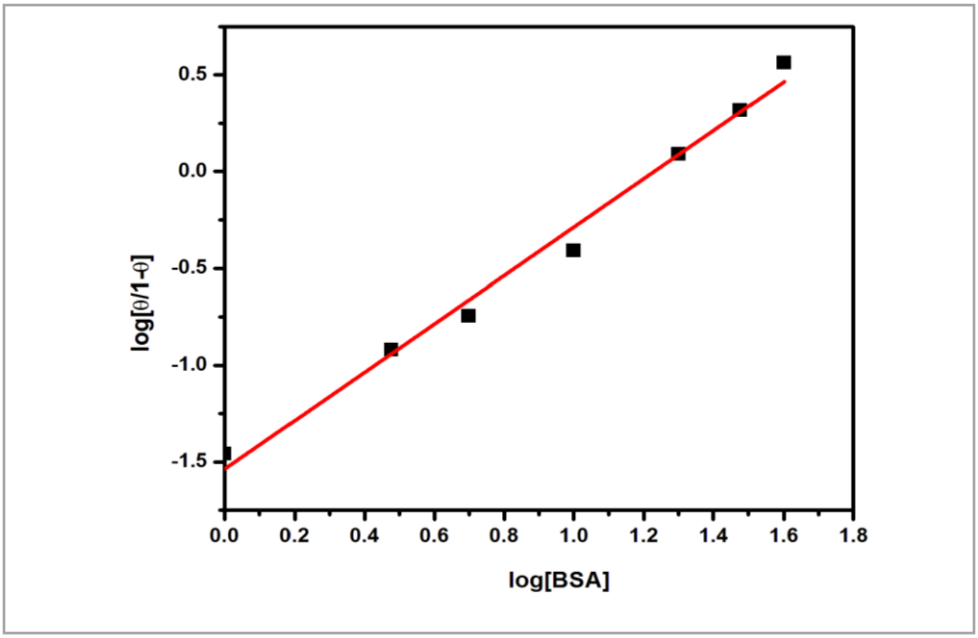

Fig. S16 1-BSA Hill's plot, where legends carry the respective meanings.

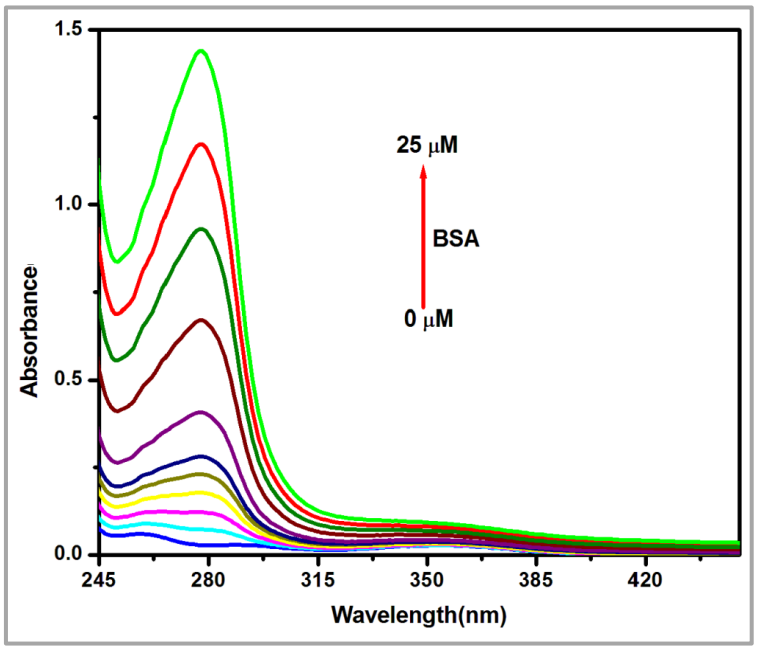

Fig. S17 UV-vis spectra of **1** (1 μM) in the presence of increasing amount of BSA (0 to 25 μM) in PBS buffer (pH = 7.4).

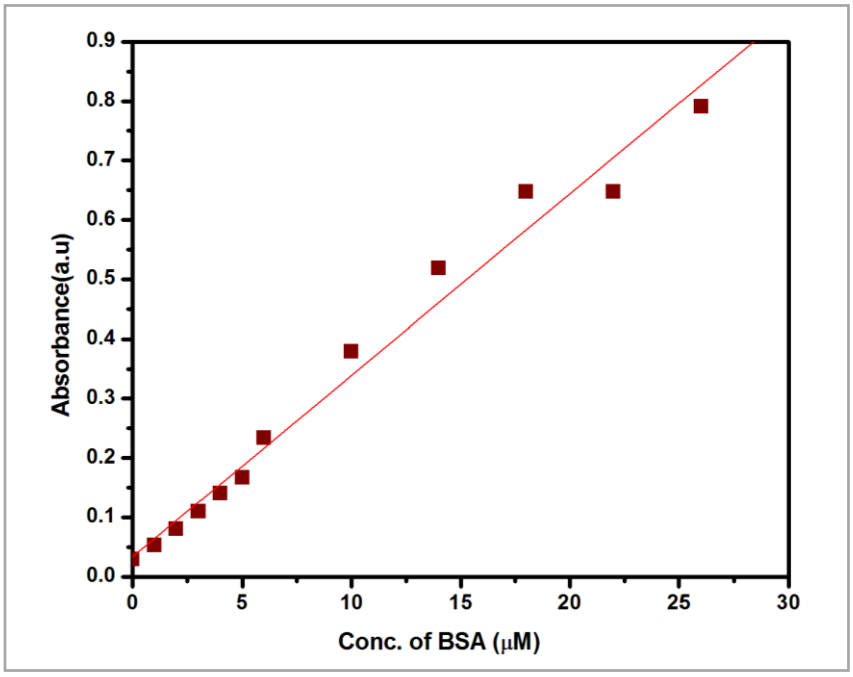

Fig. S18 The absorption of complex**1** (1 μM) at 287 nm as a function of BSA concentration.

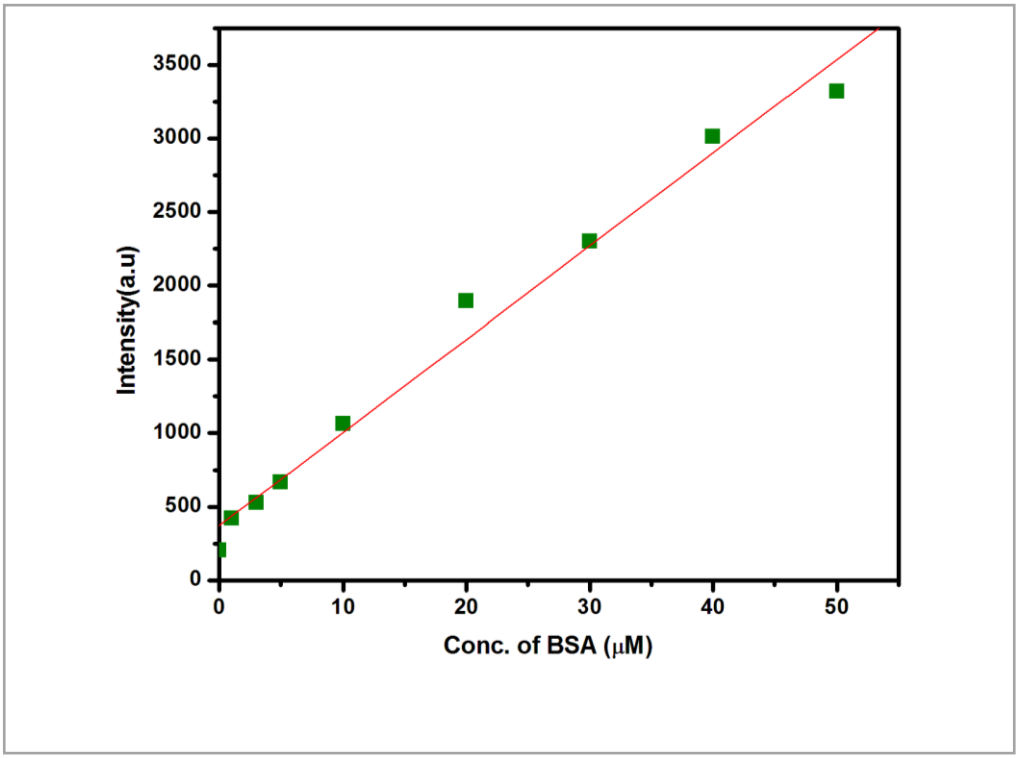

Fig. S19 The fluorescence spectra of complex**1** (0.5 μM) at 350 nm as a function of BSA concentration. (λ_{ex}=290 nm)

Table S1: Bond Lengths in Å for **1**.

Atom	Atom	Length/Å
Co	N1	2.080(3)
Co	N1[1]	2.080(3)
Co	N1[2]	2.080(3)
Co	N1[3]	2.080(3)
O1	C9	1.377(5)
O1	C30	1.428(5)
O2	C12	1.368(5)
O2	C13	1.425(5)
N1	C1	1.344(4)
N1	C5	1.343(5)
N2	C5	1.397(4)
N2	C6	1.269(4)
C1	C2	1.380(5)
C2	C3	1.379(6)
C3	C4	1.366(5)
C4	C5	1.390(5)
C6	C7	1.458(5)
C7	C8	1.400(5)
C7	C12	1.395(5)
C8	C9	1.370(5)
C9	C10	1.394(6)
C10	C11	1.375(6)
C11	C12	1.391(5)
Cl1	O3	1.417(3)
Cl1	O3[4]	1.417(3)
Cl1	O4[4]	1.425(3)
Cl1	O4	1.425(3)

--------•

[1]-1+Y,1-X,1-Z; [2]1-Y,1+X,1-Z; [3]-X,2-Y,+Z; [4]-X,1-Y,+Z

Table S2: Bond Angles in ° for **1**

Atom	Atom	Atom	Angle/°
N1	Co	N1[1]	102.07(6)
N1[1]	Co	N1[2]	125.58(15)
N1	Co	N1[2]	102.07(6)
N1	Co	N1[3]	125.58(15)
N1[3]	Co	N1[2]	102.07(6)
N1[1]	Co	N1[3]	102.07(6)
C9	O1	C30	116.5(3)
C12	O2	C13	118.3(4)
C1	N1	Co	129.0(2)
C5	N1	Co	112.4(2)
C5	N1	C1	118.6(3)
C6	N2	C5	119.8(3)
N1	C1	C2	122.1(3)
C3	C2	C1	118.5(4)
C4	C3	C2	120.2(4)
C3	C4	C5	118.3(4)
N1	C5	N2	112.1(3)
N1	C5	C4	122.1(3)
C4	C5	N2	125.7(3)
N2	C6	C7	121.0(3)
C8	C7	C6	119.2(3)
C12	C7	C6	120.7(4)
C12	C7	C8	120.0(4)
C9	C8	C7	120.2(4)
O1	C9	C10	116.1(3)
C8	C9	O1	124.4(4)
C8	C9	C10	119.4(4)
C11	C10	C9	121.3(4)
C10	C11	C12	119.6(4)
O2	C12	C7	115.6(4)
O2	C12	C11	124.8(4)
C11	C12	C7	119.5(4)
O3	Cl1	O3[4]	110.9(3)
O3	Cl1	O4	111.0(2)
O3[4]	Cl1	O4[4]	111.0(2)
O3[4]	Cl1	O4	108.5(2)
O3	Cl1	O4[4]	108.5(2)
O4[4]	Cl1	O4	107.1(3)

-------•

[1]1-Y,1+X,1-Z; [2]-1+Y,1-X,1-Z; [3]-X,2-Y,+Z; [4]-X,1-Y,+Z