Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

A triple action chemosensor for Cu^{2+} by chromogenic, Cr^{3+} by fluorogenic and CN^- by relay recognition method with bio-imaging of HeLa cells

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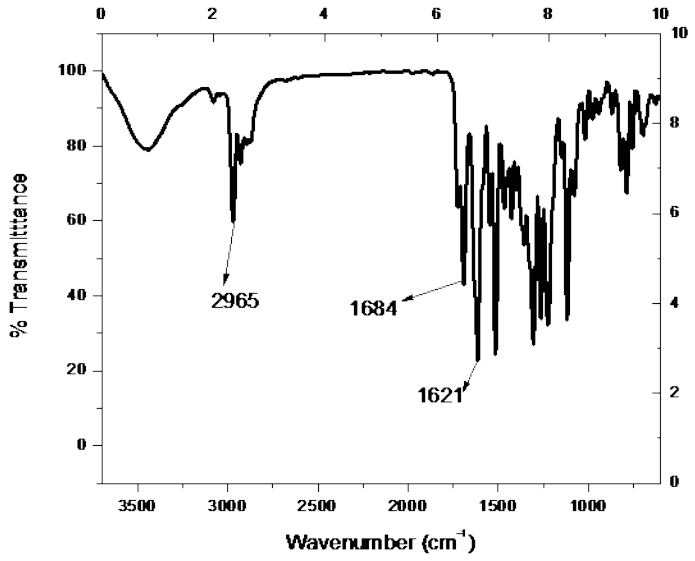
Supporting information

Fig. S1. FT-IR spectrum of **R1**



2965 (-C-H); 1684 (C=O, carbonyl); 1621 (C=N, azomethine)

Fig. S2. ^{1}H NMR spectrum of **R1**

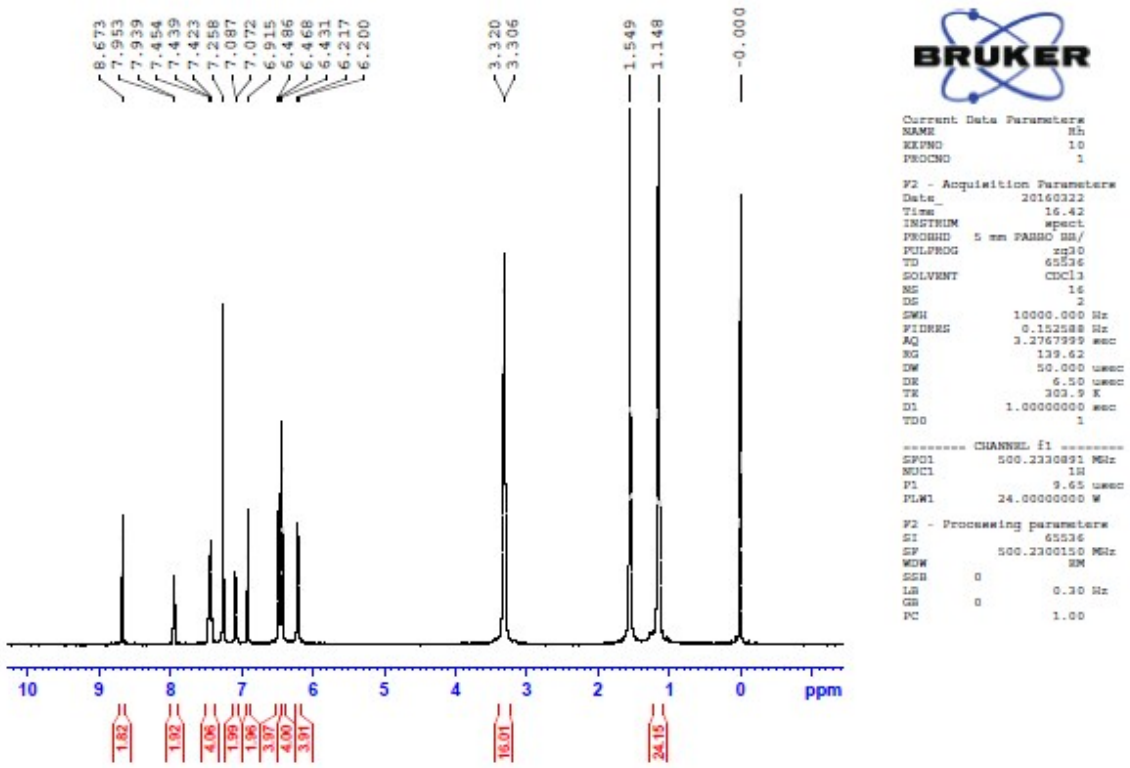
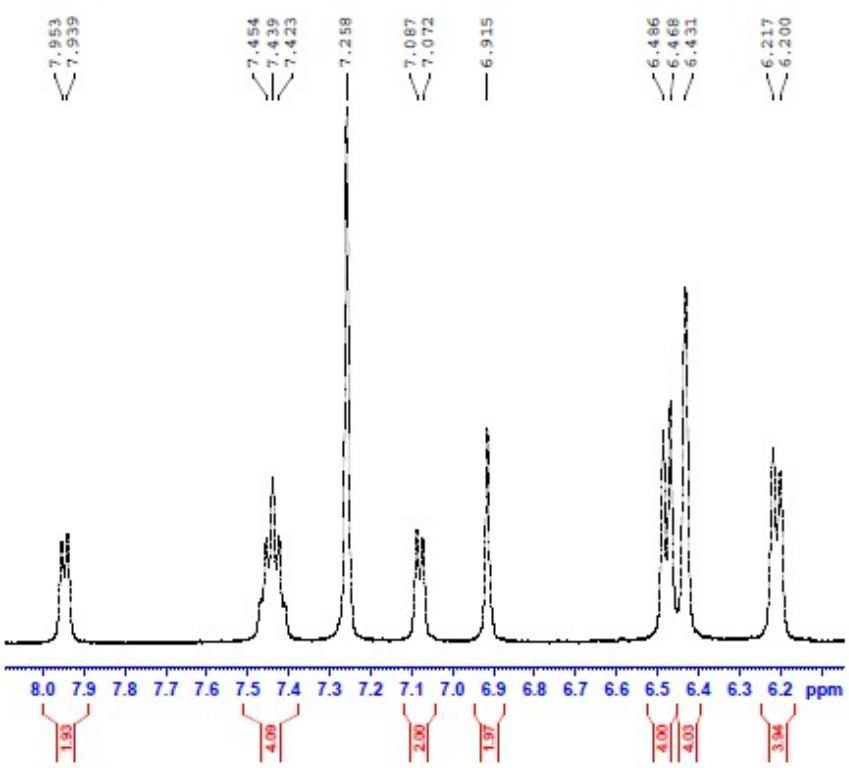


Fig. S3. ^{1}H NMR of **R1** (expansion)



BRUKER

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EXPNO                 10
PROCNO                 1

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PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              10000.000 Hz
FIDRES               0.152588 Hz
AQ                3.2767999 sec
RG                   139.62
DW                   50.000 usec
DE                    6.50 usec
TE                   303.9 K
D1                1.00000000 sec
TD0                      1

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NUC1                    1H
P1                     9.65 usec
PLW1            24.00000000 W

F2 - Processing parameters
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WDW                     EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
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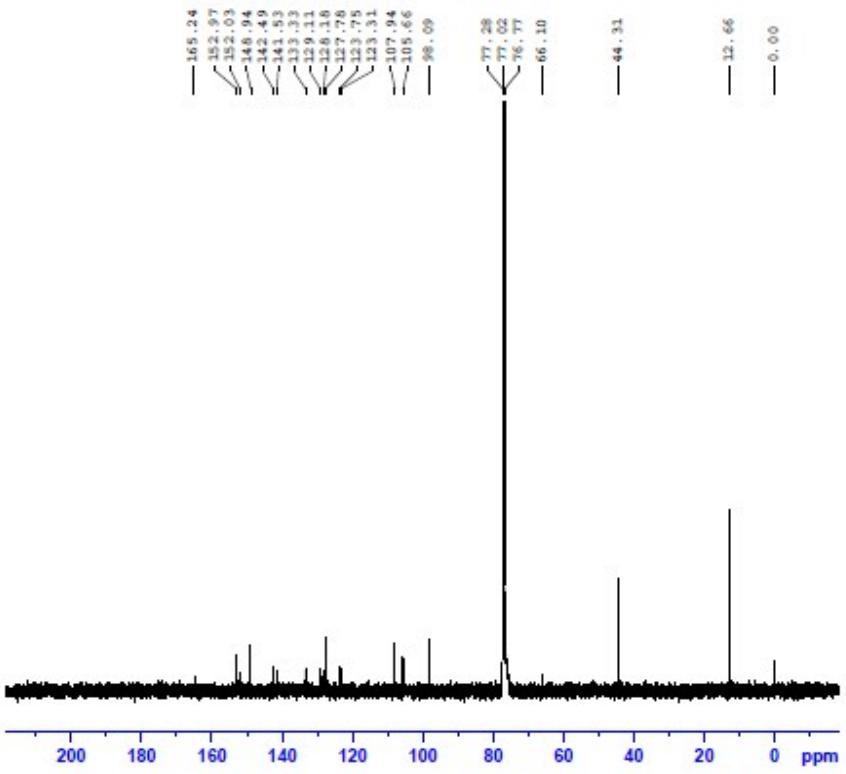
Fig. S4. ^{13}C NMR of **R1**

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PROCNO                     1

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TD                 65536
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NS                 1024
DS                 4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                 192.47
DW                 16.800 usec
DE                 6.50 usec
TE                 297.9 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                        1

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NUC1                    13C
P1                    9.50 usec
PLW1           91.00000000 W

======== CHANNEL f2 ========
SFO2           500.2320009 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                80.00 usec
PLW2           24.00000000 W
PLW12           0.34200999 W
PLW13           0.21889000 W

F2 - Processing parameters
SI                     32768
SF             125.7829335 MHz
WDW                       EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
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Fig. S5. HRMS of **R1**

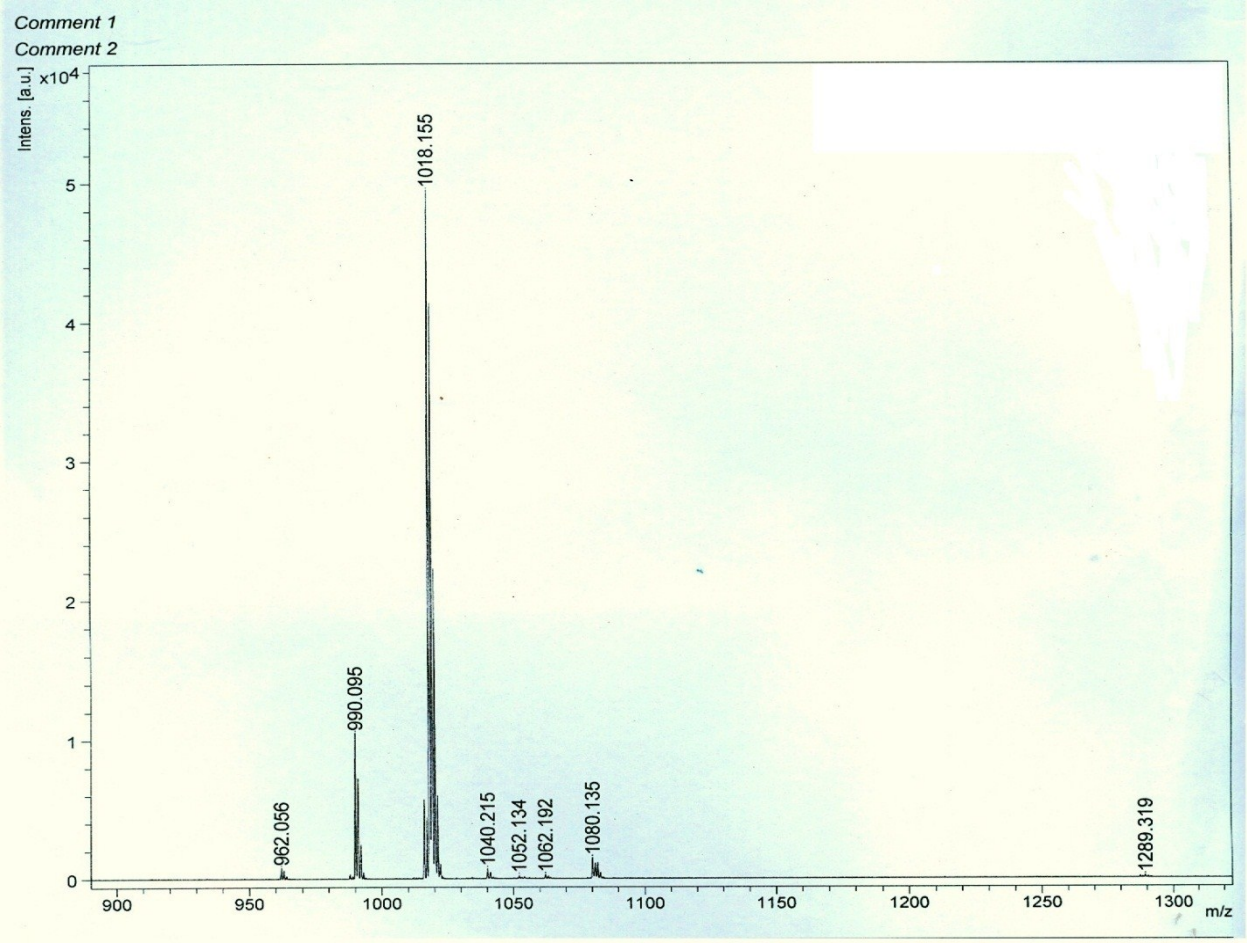
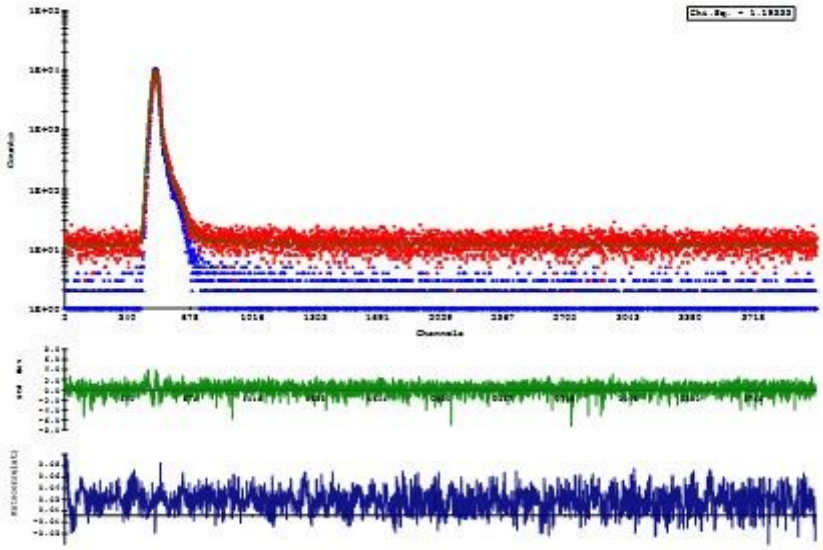


Fig. S6. Life time measurement of **R1**



```
Calculated using 2 exponentials

Prompt data : Prompt
Decay data : r12

The initial parameters are:

 Shift Value = 0        ch;          0               sec
 Shift Limit = 40       ch;          2.194757E-09    sec

 I1 Estimate = 0.0995   ch;          5.459534E-12    sec
 I2 Estimate = 0.595    ch;          2.185814E-11    sec

 A Free
 B1 Free
 B2 Free

 Prompt and decay LO = 2      ch;    1.097394E-10    sec
 Prompt and decay HI = 4096   ch;    2.247462E-07    sec

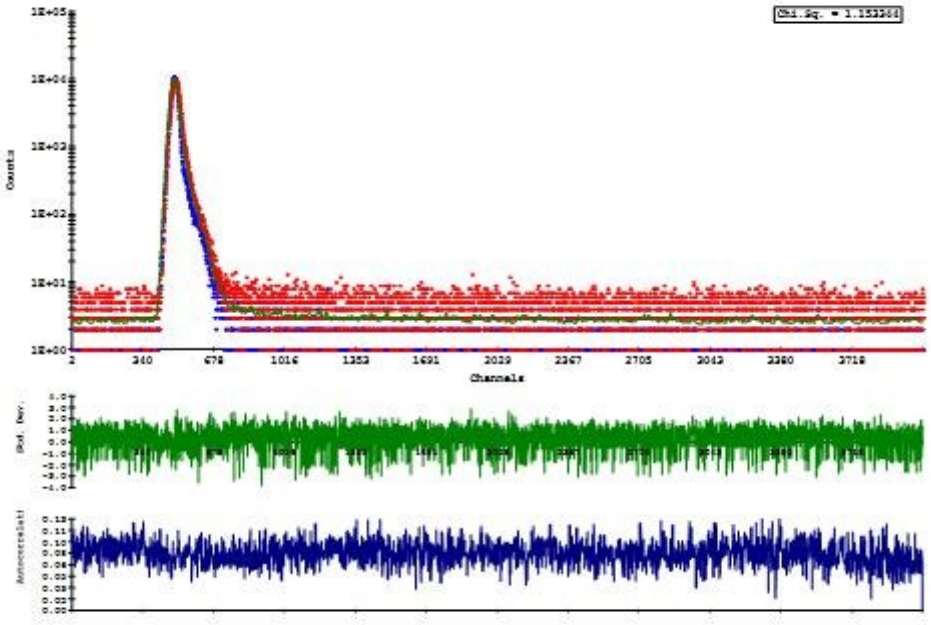
 Background on prompt = 1.149035
 Time calibration = 5.456969E-11 sec/ch

The fitted parameters are:

 Hi reduced to: 4056 ch

 SHIFT = -5.50435      ch;    -3.020222E-10  sec     S.Dev = 1.987764E-12  sec
 I1    = 5.673416      ch;    3.112957E-10   sec     S.Dev = 5.594208E-12  sec
 I2    = 40.27925      ch;    2.21011E-09    sec     S.Dev = 7.669781E-11  sec
 A     = 11.66975                                   S.Dev = 5.710542E-02
 B1    = 0.1555812     [ 95.65 Rel.Ampl][ 0.99 Alpha] S.Dev = 4.061218E-04
 B2    = 1.190541E-03  [ 4.35 Rel.Ampl][ 0.01 Alpha] S.Dev = 2.571613E-03
Average Life Time = 3.233559E-10  sec
CHISQ = 1.19333              [ 4049 degrees of freedom ]
```

Fig. S7. Life time measurement of **R1**+Cr^{3+}




```
Calculated using 2 exponentials

Prompt data : Prompt
Decay data : r12 cr3+

The initial parameters are:

 Shift Value = 0        ch;          0              sec
 Shift Limit = 40       ch;          2.194787E-09   sec

 T1 Estimate = 0.0995   ch;          5.459534E-12   sec
 T2 Estimate = 0.395    ch;          2.183514E-11   sec

 A Free
 B1 Free
 B2 Free

 Prompt and decay LO = 2      ch;    1.097384E-10   sec
 Prompt and decay HI = 4096   ch;    2.247462E-07   sec

 Background on prompt = 1.149035
 Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

 Hi reduced to: 4056 ch

 SHIFT = -3.42549       ch;    -1.879555E-10 sec      S.Dev = 2.268572E-12   sec
 T1    = 9.026775       ch;    4.952963E-10  sec      S.Dev = 1.572668E-11   sec
 T2    = 25.70676       ch;    1.410522E-09  sec      S.Dev = 4.353468E-11   sec
 A     = 2.254145                                     S.Dev = 2.766171E-02
 B1    = 0.1125443      [ 88.27 Rel.Ampl][ 0.96 Alpha] S.Dev = 3.505148E-04
 B2    = 5.265145E-03   [ 11.73 Rel.Ampl][ 0.04 Alpha] S.Dev = 9.53555E-05
 Average Life Time = 3.360857E-10  sec
 CHISQ = 1.153344            [ 4049 degrees of freedom ]
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Fig. S8. Job's plot of Cr^{3+}

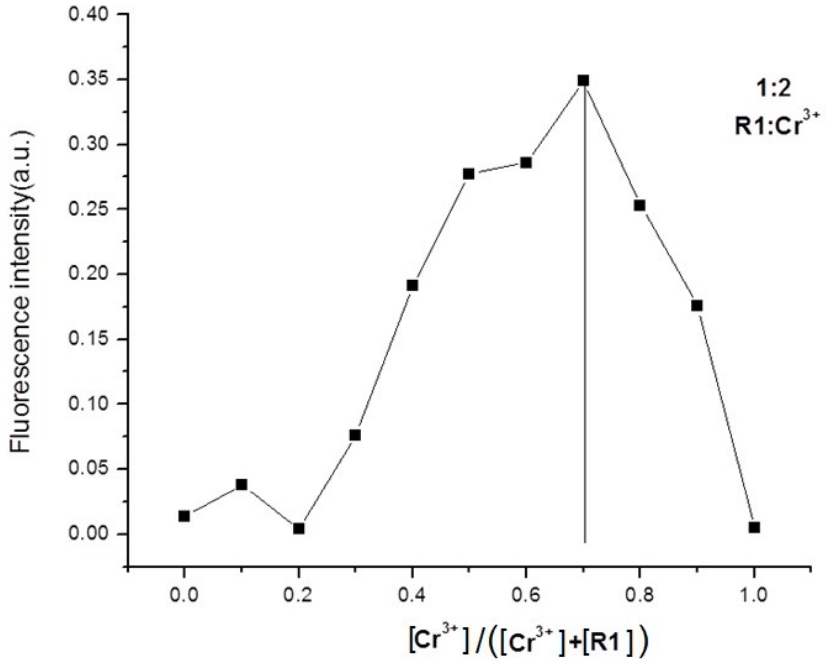


Fig. S9. Job's plot of Cu^{2+}

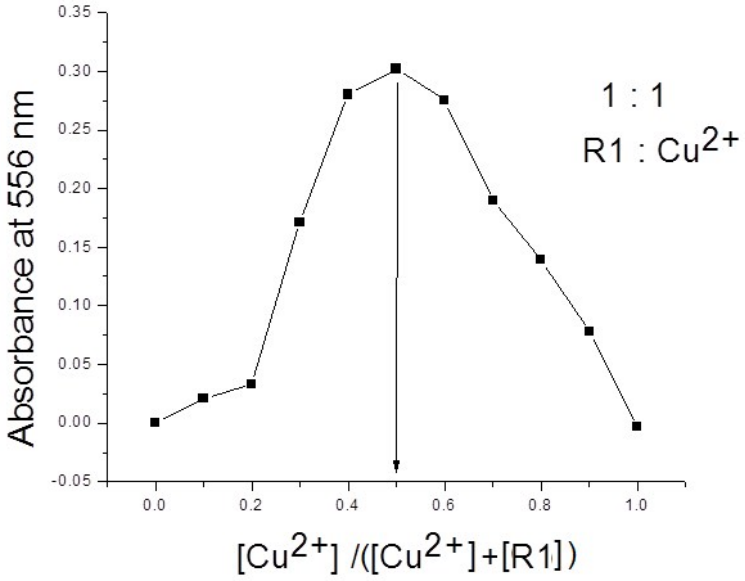
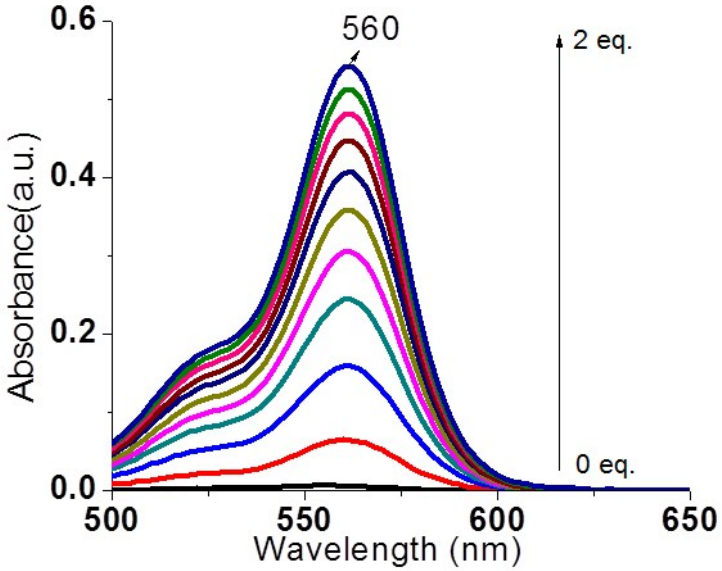
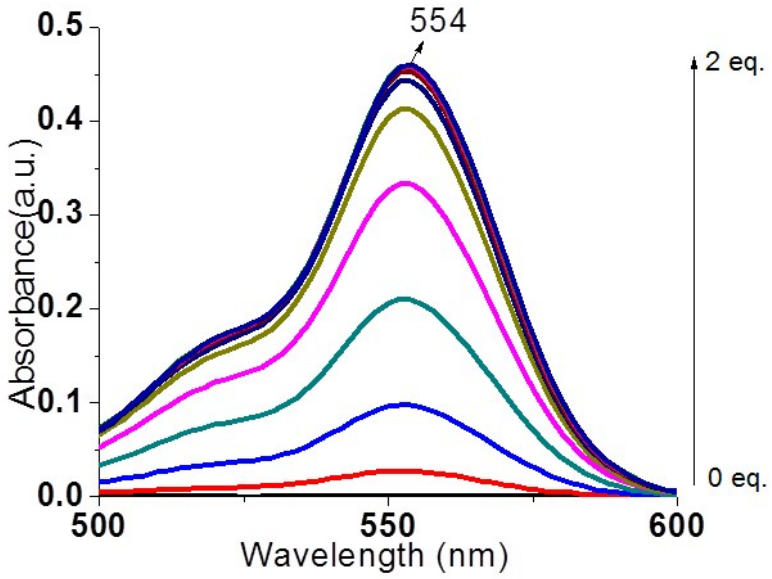


Fig. S10. Absorption spectrum of R1 upon incremental addition of Cr^{3+}



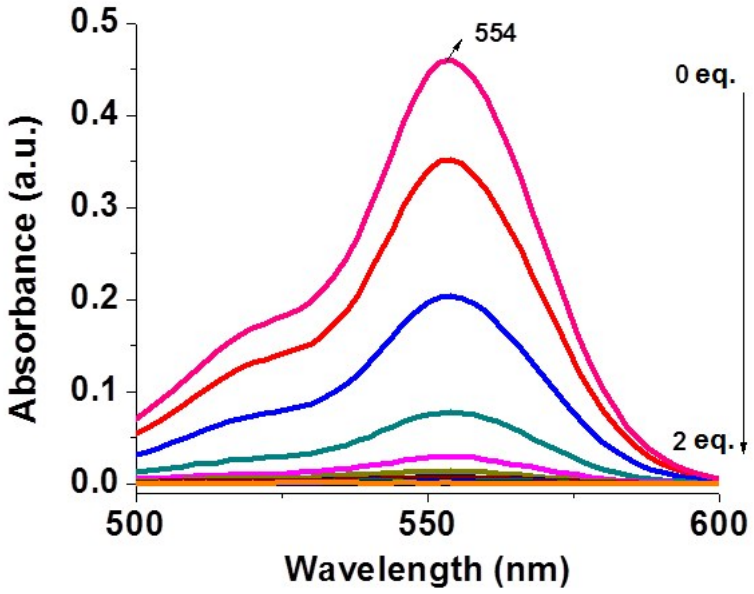
Changes in the absorption of **R1** (50 μM) in $CH_3CN–H_2O$ (4:1, v/v) with increasing concentrations of Cr^{3+} in H_2O (0–2 eq.).

Fig. S11. Absorption spectrum of R1 upon incremental addition of Cu^{2+}



Changes in the absorption of **R1** (50 μM) in $CH_3CN–H_2O$ (4:1, v/v) with increasing concentrations of Cu^{2+} in H_2O (0–2 eq.).

Fig. S12. Absorption spectrum of R1 upon incremental addition of CN^-



Changes in the absorption of **R1** (50 μM) with Cu^{2+} (2 eq.) in $CH_3CN–H_2O$ (4:1, v/v) with increasing concentrations of CN^- in H_2O (0–2 eq.).

Fig. S13 (a) Benesi-Hildebrand plot of **R1** with Cr^{3+} and **(b)** Plot of absorbance versus concentration of Cr^{3+}

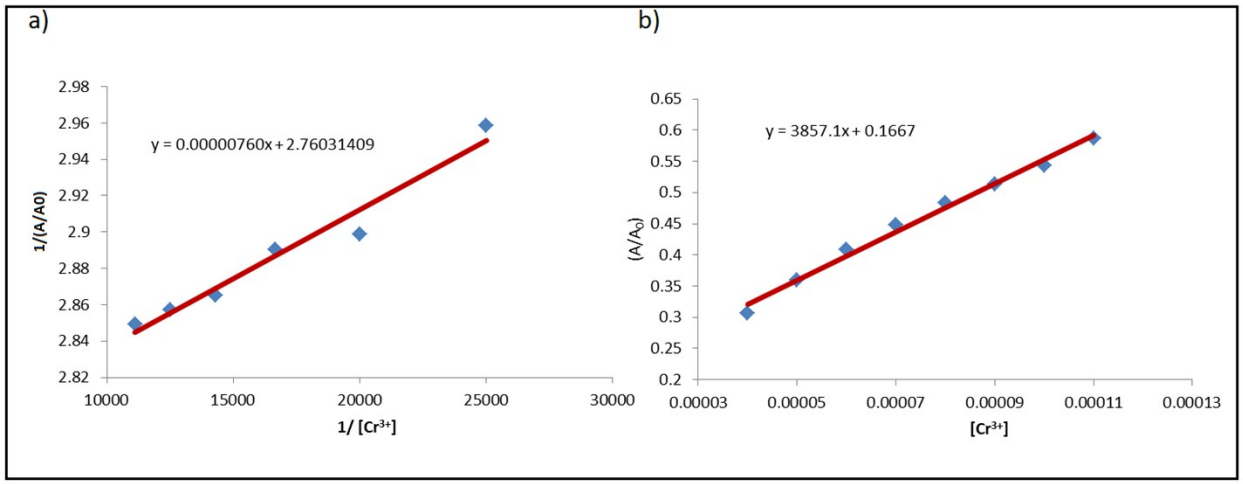


Fig. S14. (a) Benesi-Hildebrand plot of **R1** with Cu^{2+} and **(b)** Plot of absorbance versus concentration of Cu^{2+}

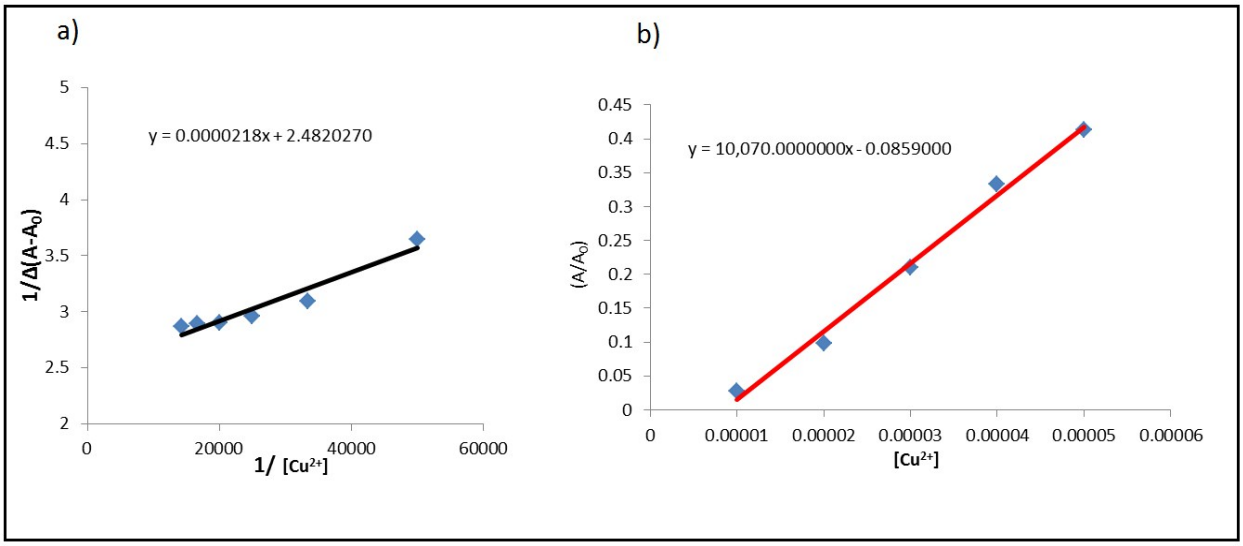


Fig. S15. (a) Benesi-Hildebrand plot of **R1** with CN^- and **(b)** Plot of absorbance versus concentration of CN^-

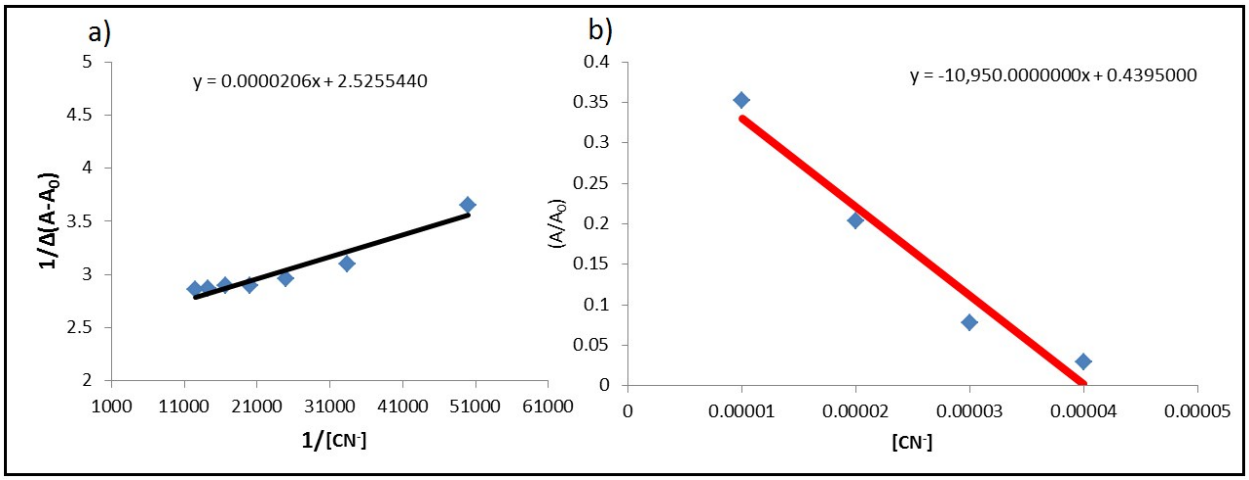
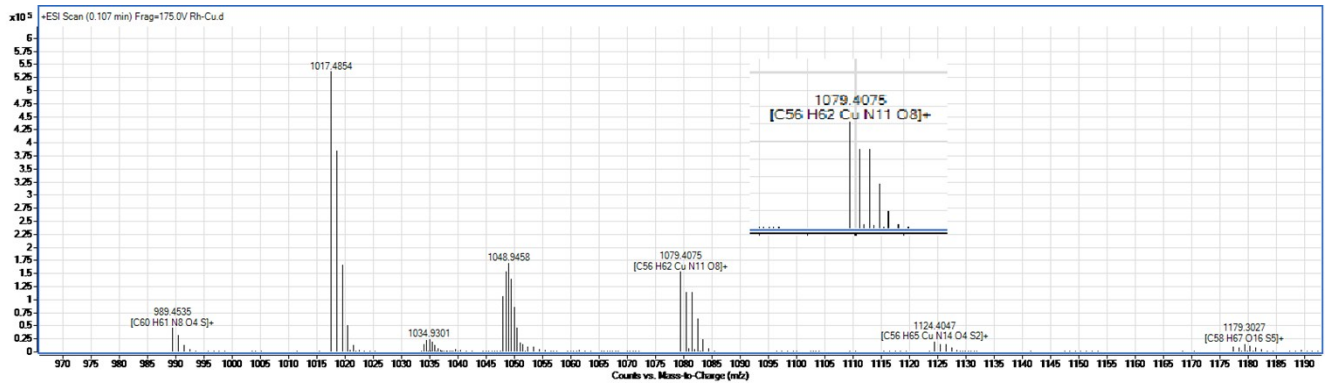


Fig. S16. ESI mass datum of **R1**-Cu^{2+}complex



R1-Cu^{2+}, calculated mass:1079, mass obtained:1079.4075

Fig. S17. ESI mass datum of **R1**-Cu^{2+}+CN^- complex

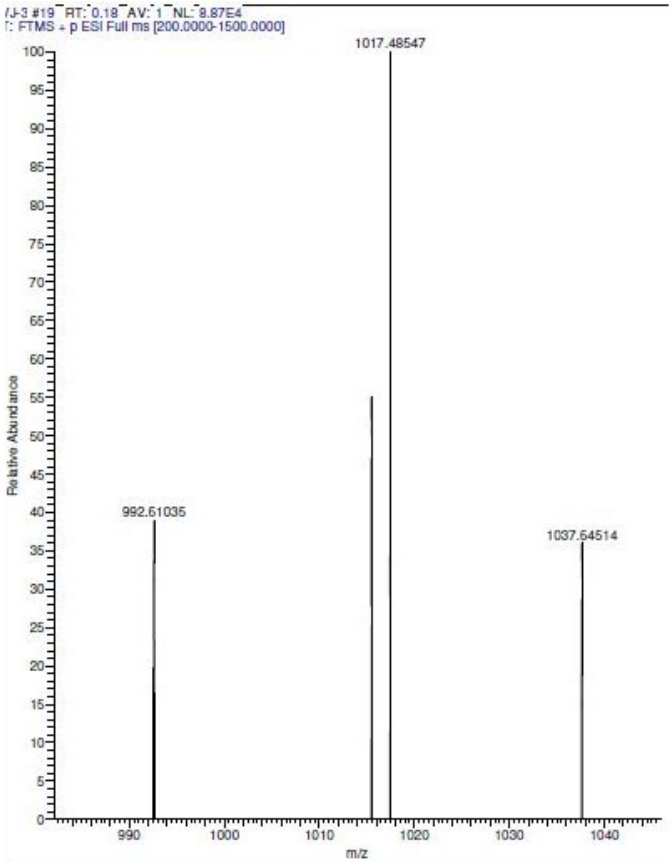
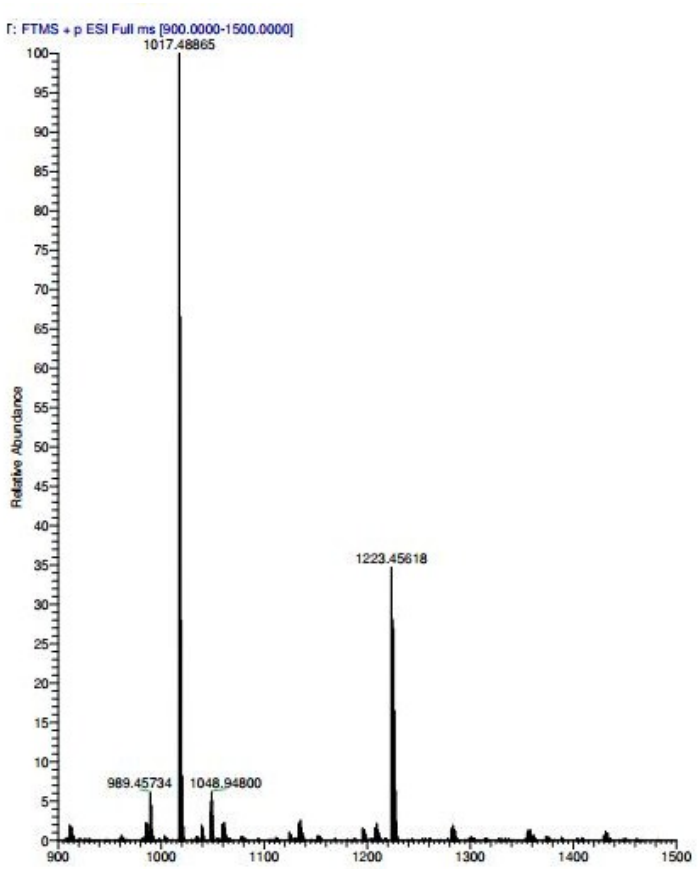


Fig. S18. ESI mass datum of **R1**-Cr^{3+}complex



Calculated mass:1222, mass obtained:1223.45618 (m+1). Mass spectrum taken in MeOH medium.

R1-Cr_2+Cl_2+MeOH peak interpretation done according to the reference cited 53.