Synthesis of η^5-C_5H_4R based compounds with functional moieties for sensing and imaging applications.

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Sandwich

Half Sandwich

Ferrocenyl based system

Ferrocenyl – heterocycle system

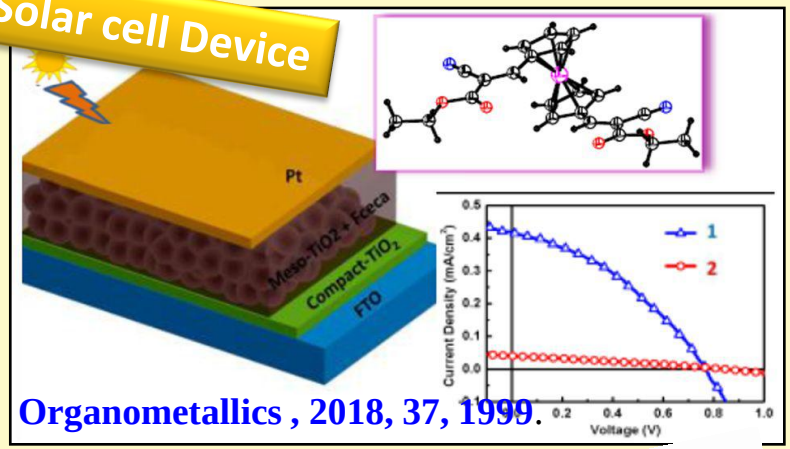
Cymantrenyl– heterocycle system

Bifunctional Diferrocenyl system

Ferroceneyl – Half sandwich based

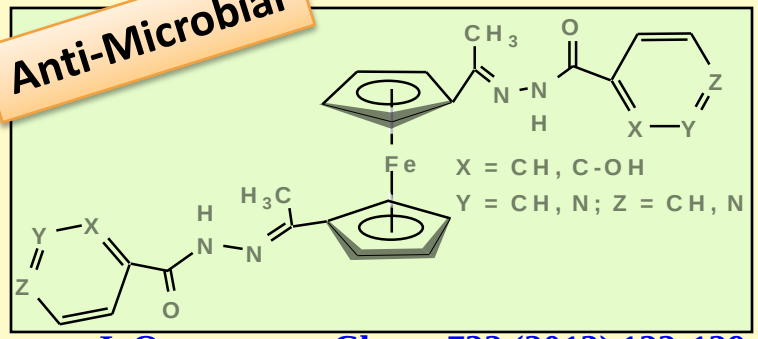
Ferrocene based Multimetallic clusters

Solar cell Device



Organometallics , 2018, 37, 1999.

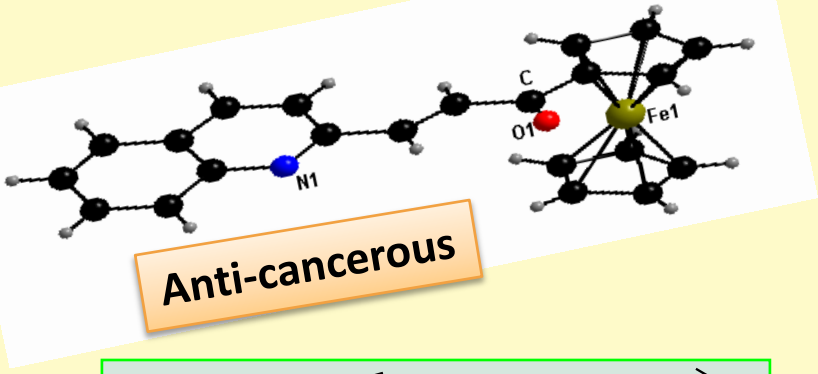
Anti-Microbial



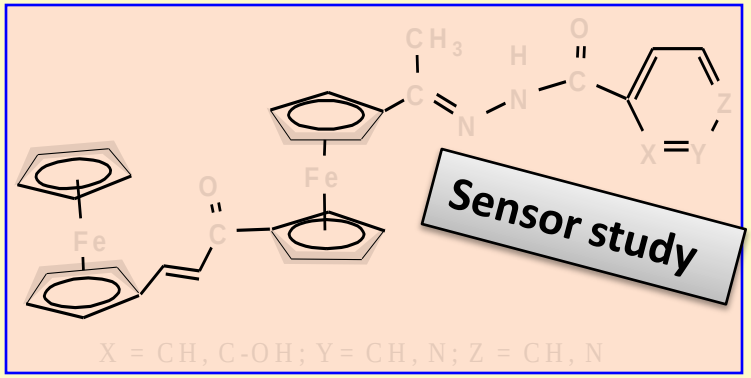
J. Organomet. Chem. 732 (2013) 122-129.

J. Mol. Str. , 2015, 1085, 162.

Anti-cancerous

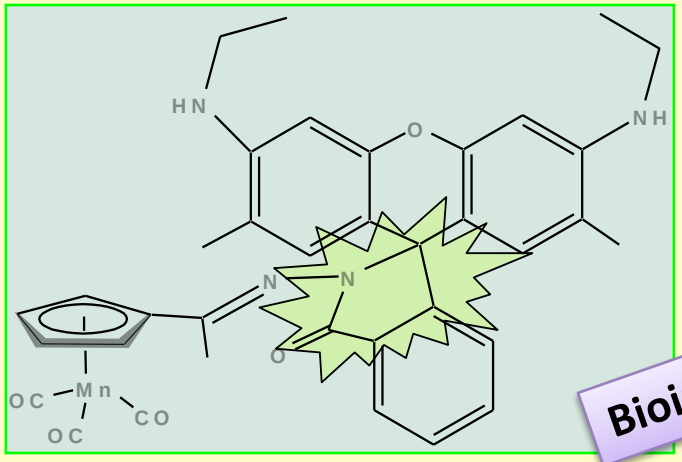


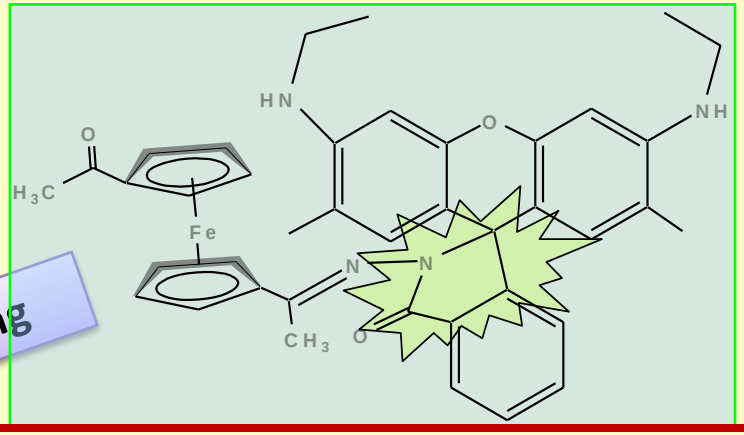
Sensor study

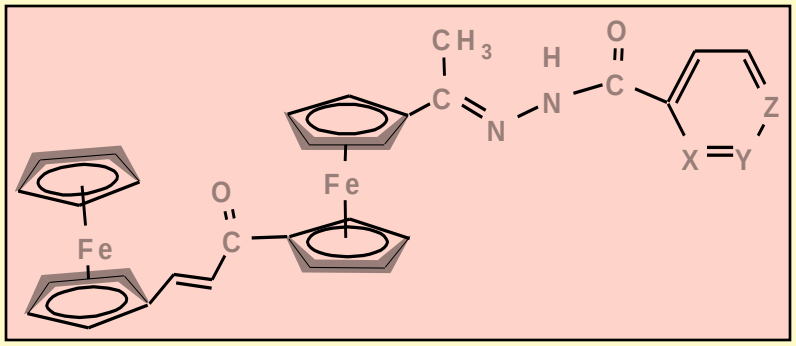


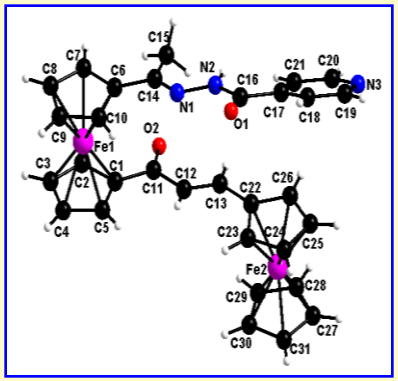
Eur. J. Inorg. Chem. 2016, 5485

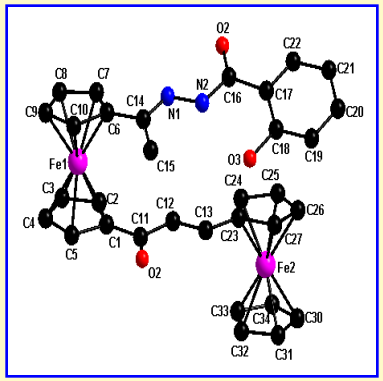
Bioimaging

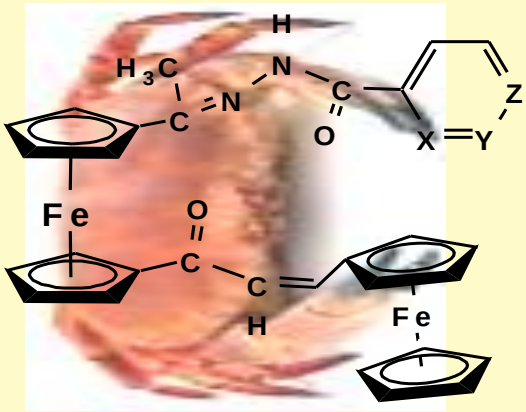




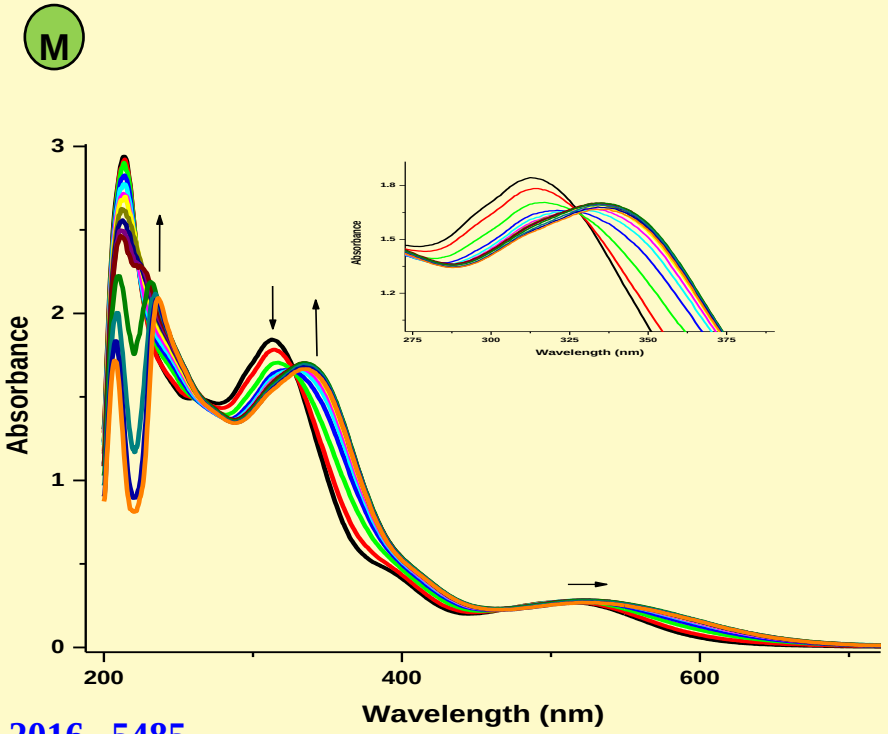






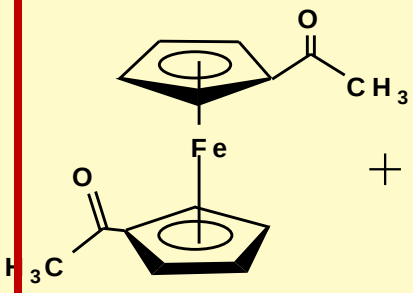


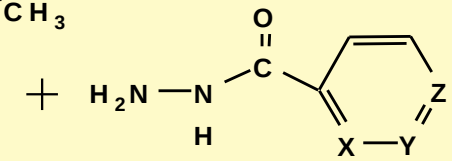
Selectively binds Pb^{2+} cation



Eur. J. Inorg. Chem. 2016, 5485

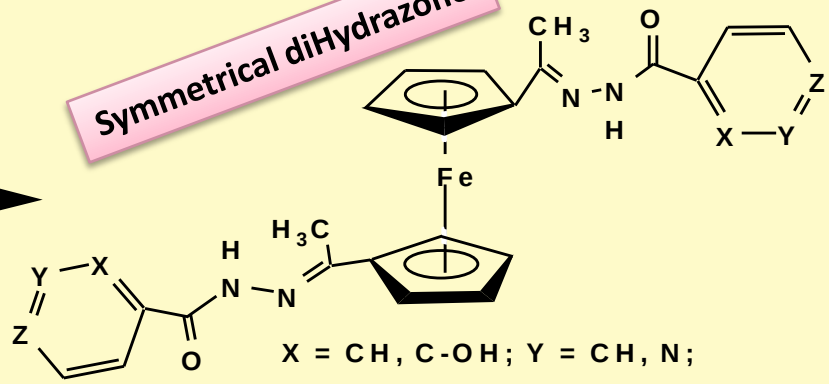
Selective Functionalization :





X = CH, C-OH; Y = CH, N;
Z = CH, N

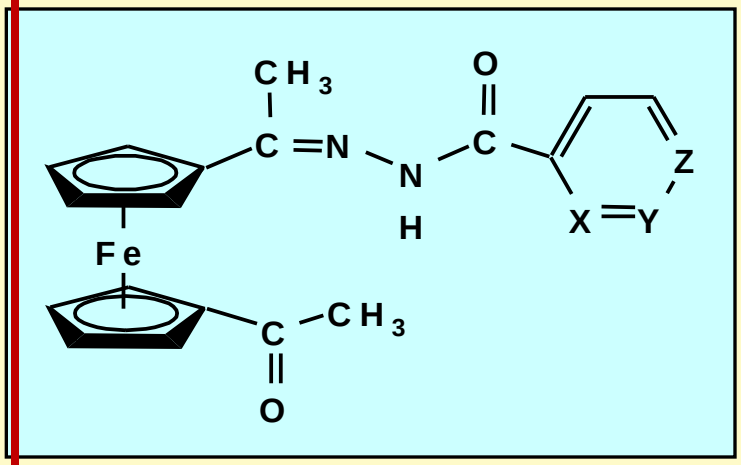
Symmetrical diHydrazone



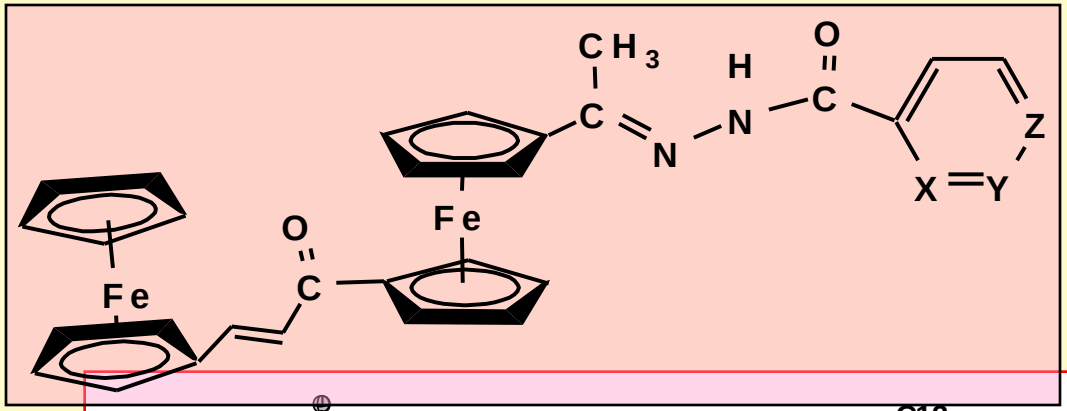
X = CH, C-OH; Y = CH, N;
Z = CH, N

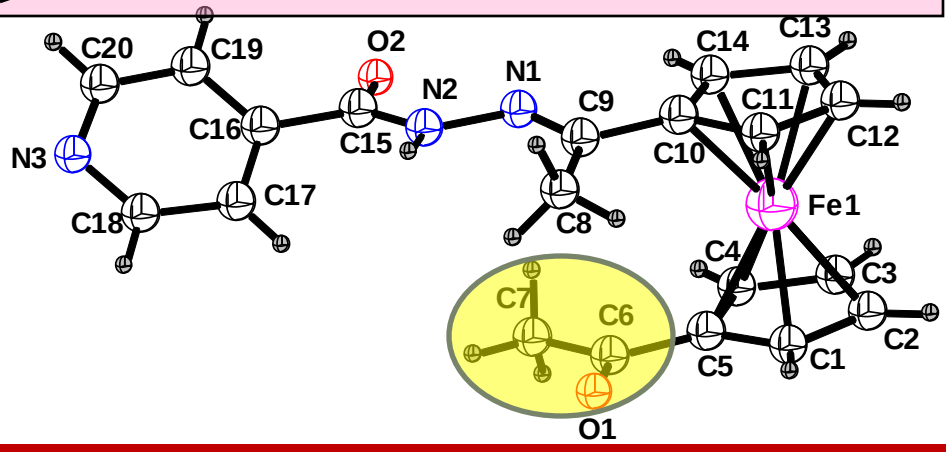
High antibacterial activity !!

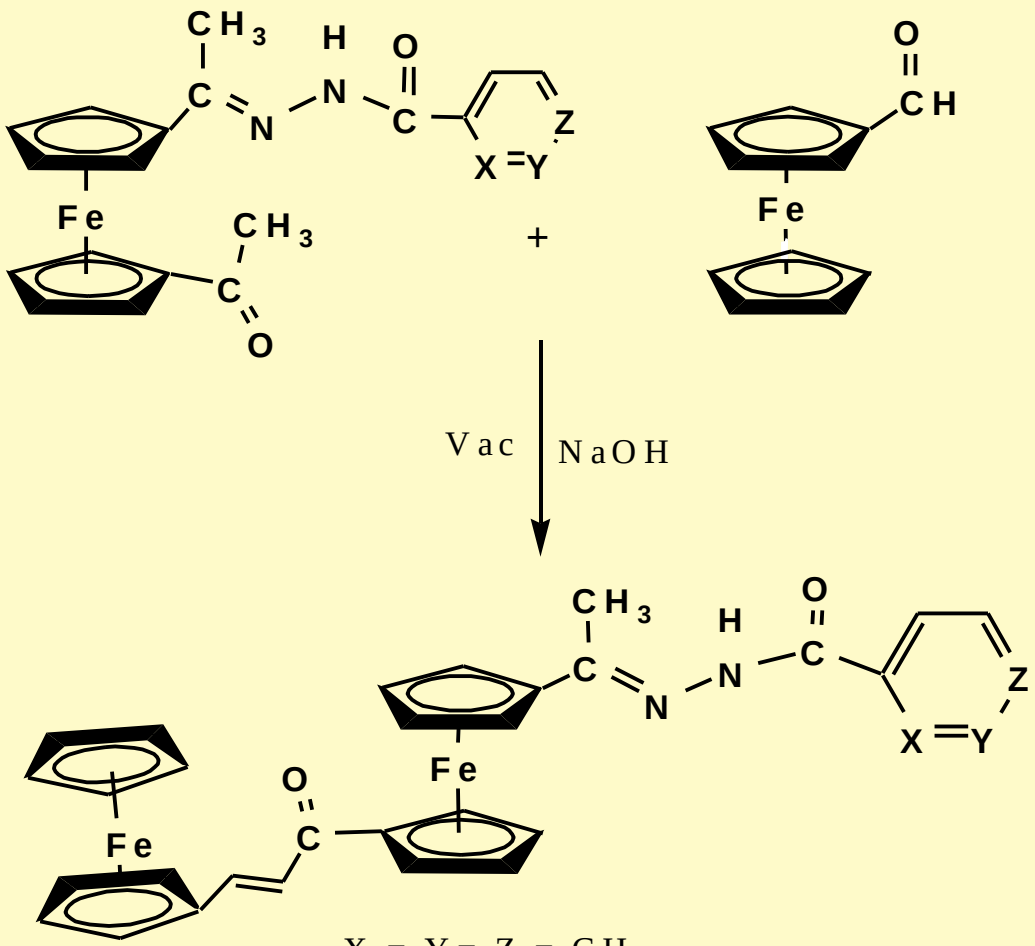
Rice Husk Silica



Only product







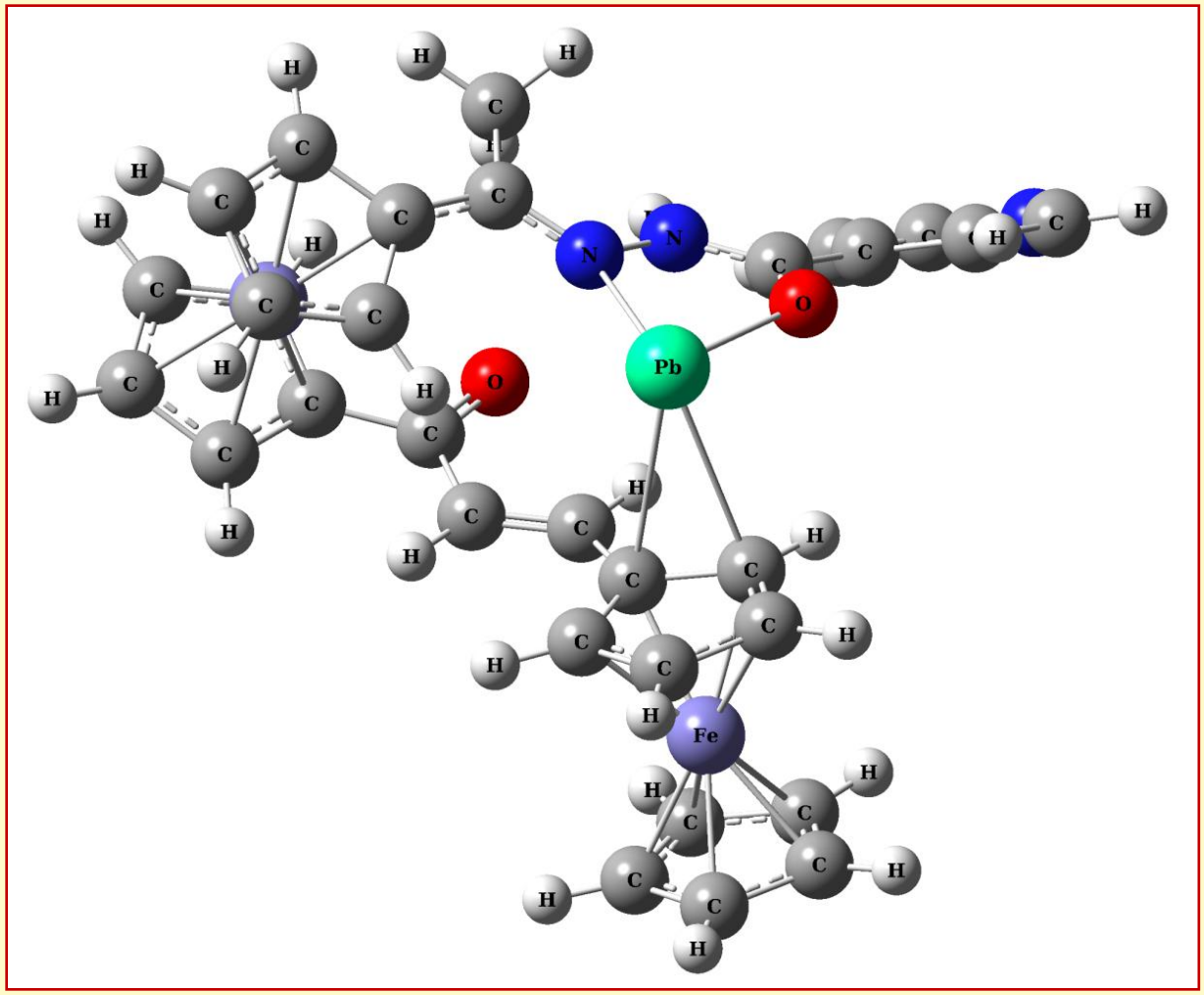
X = Y = Z = CH

X = C-OH, Y = Z = CH

X = Z = CH, Y = N

X = Y = CH, Z = N

Optimized geometry of Pb^{2+} complex

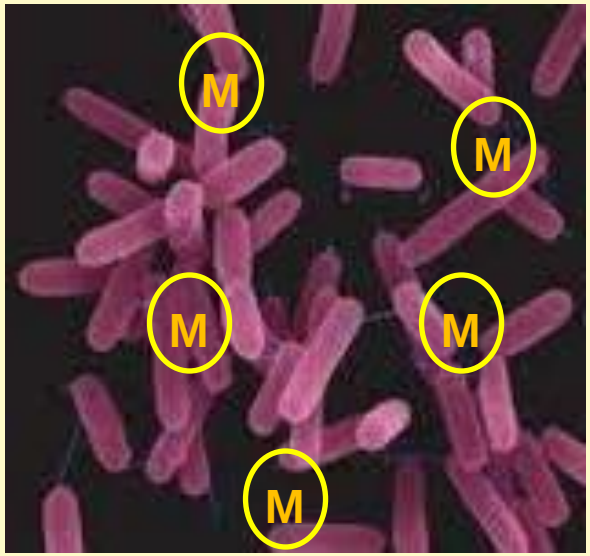


Pb –O = 2.28 Å ; Pb – N = 2.52 Å ; Pb – C(Cp) = 2.84 Å

M^{2+} sensing prompted us to evaluate more such compounds but with a fluorescent probe and to use them in biological medium , particularly in bacterial and cancer cells.

Bacterial Uptake of Metal ions

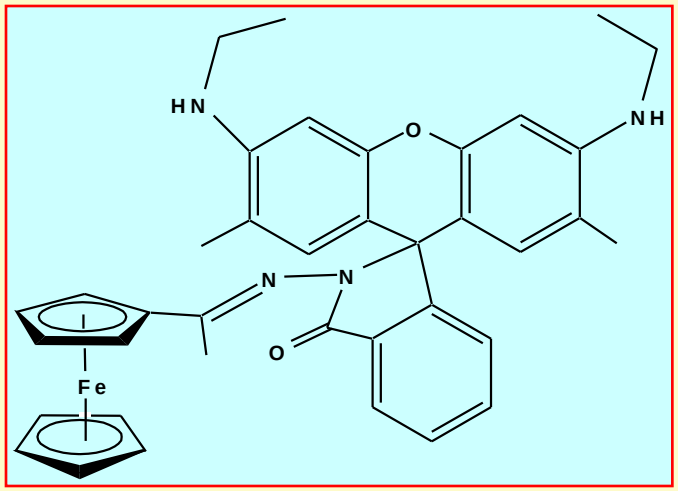
Complex uptake Mechanism !!!



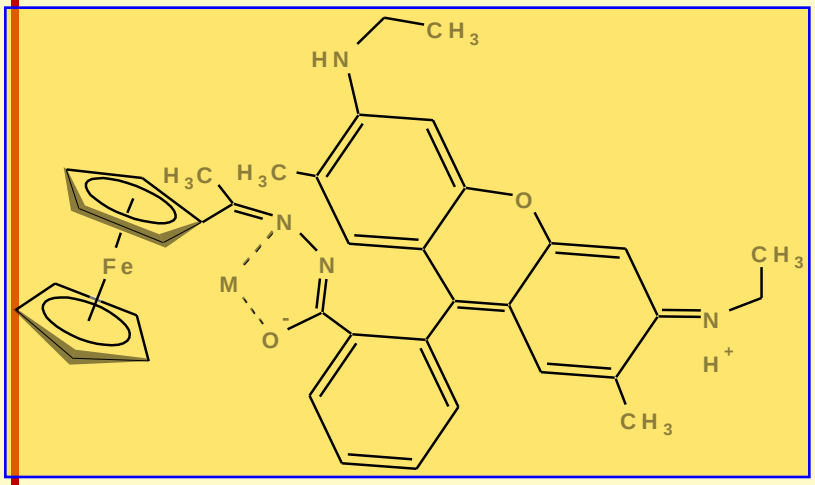
Metal ions are essential for Microorganisms during the process of infection and are involved in bacterial metabolism and various virulance factor function

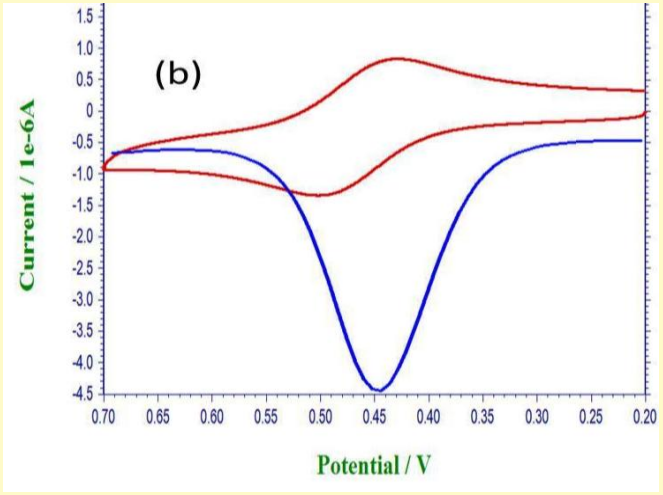
But the complexity by which these prokaryots interact with metal ions and act during infection are poorly understood and under investigation by various group.

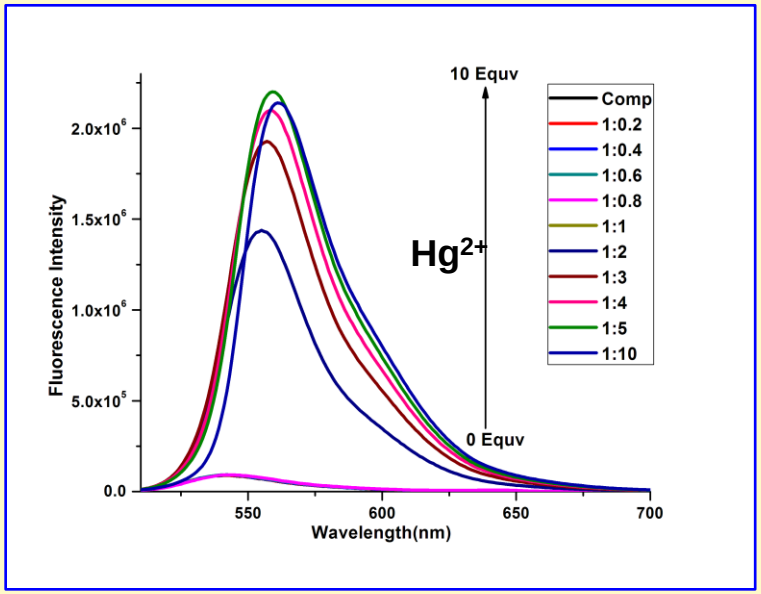
Sandwich fluorescent hydrazone:



M^{2+}

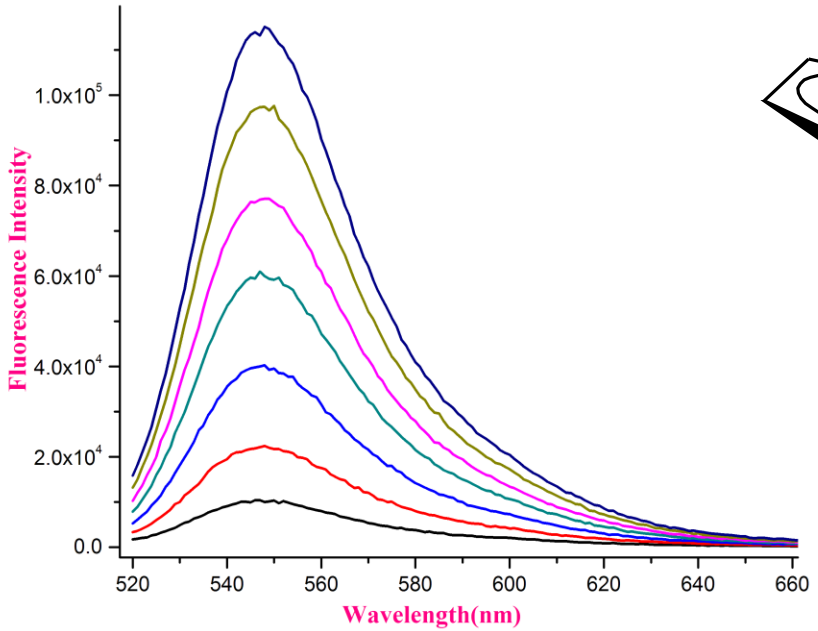


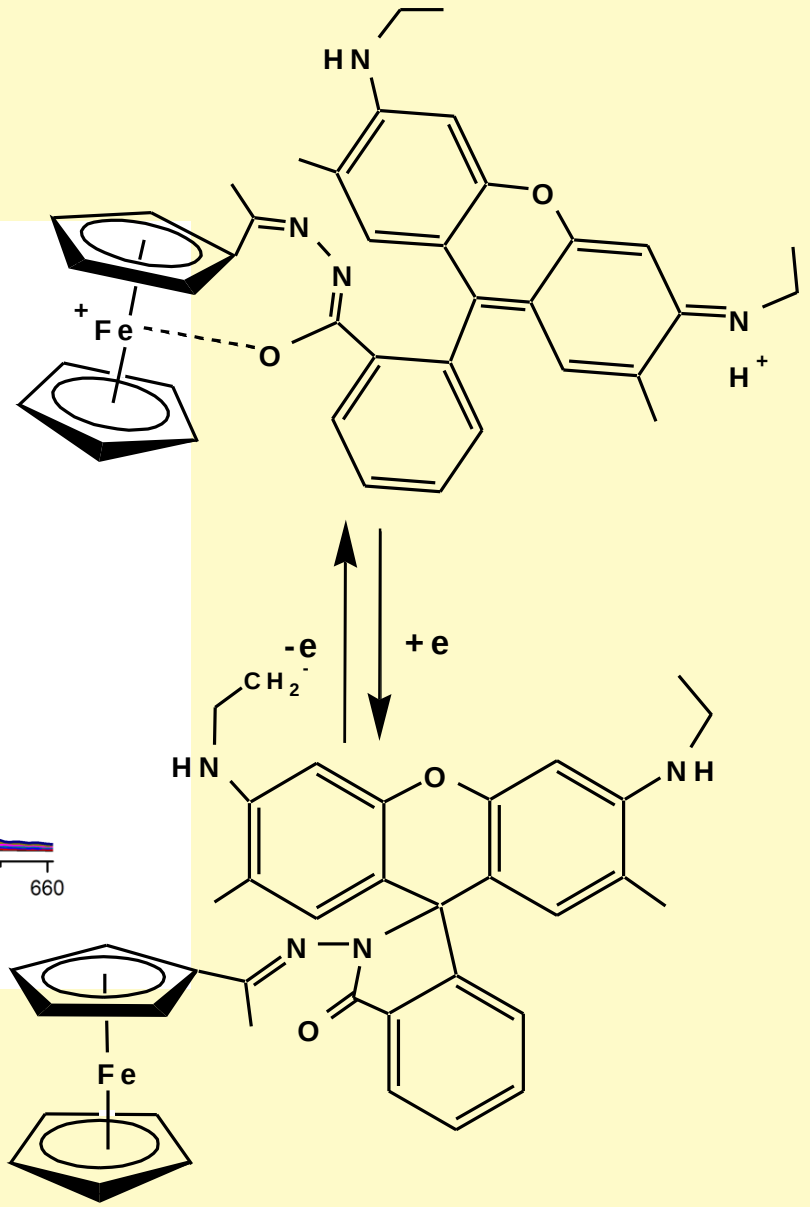


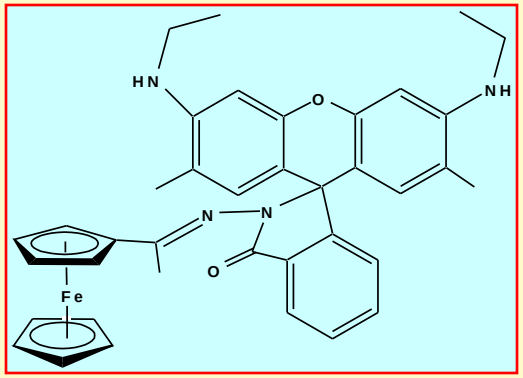


Zn^{2+} and Cd^{2+} also showed interaction

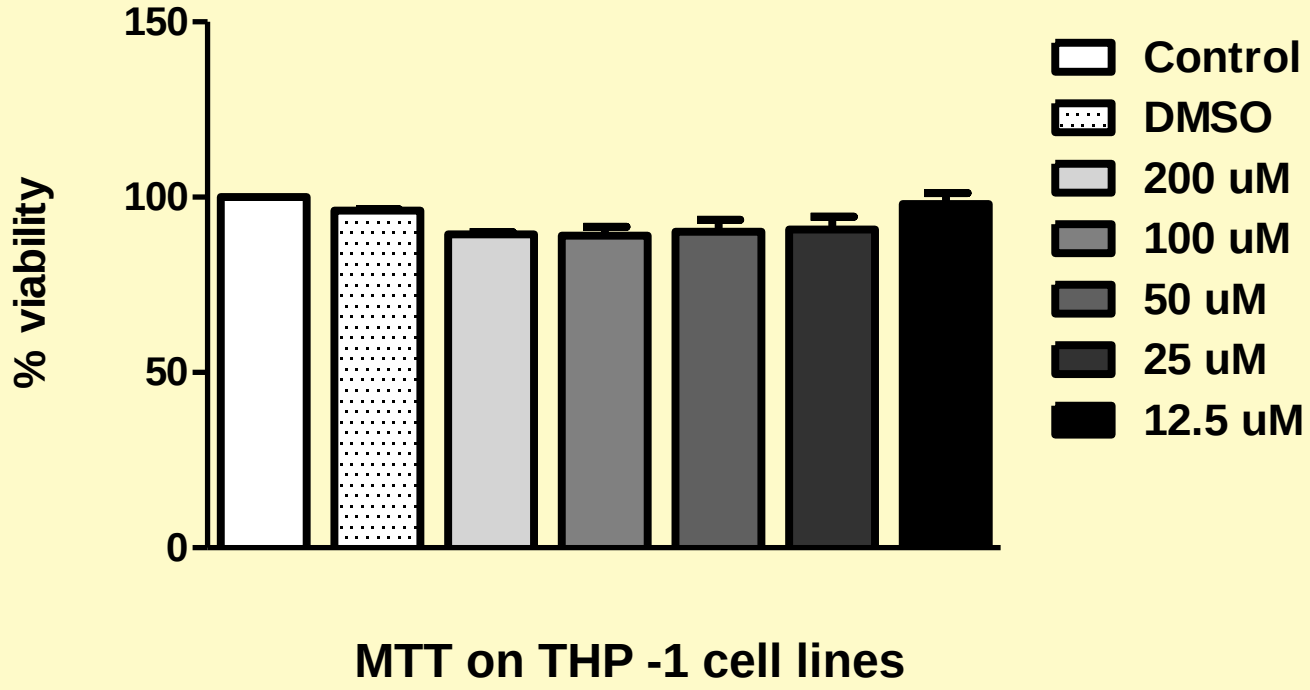
Redox Switch :

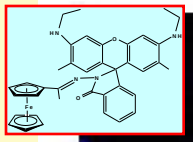




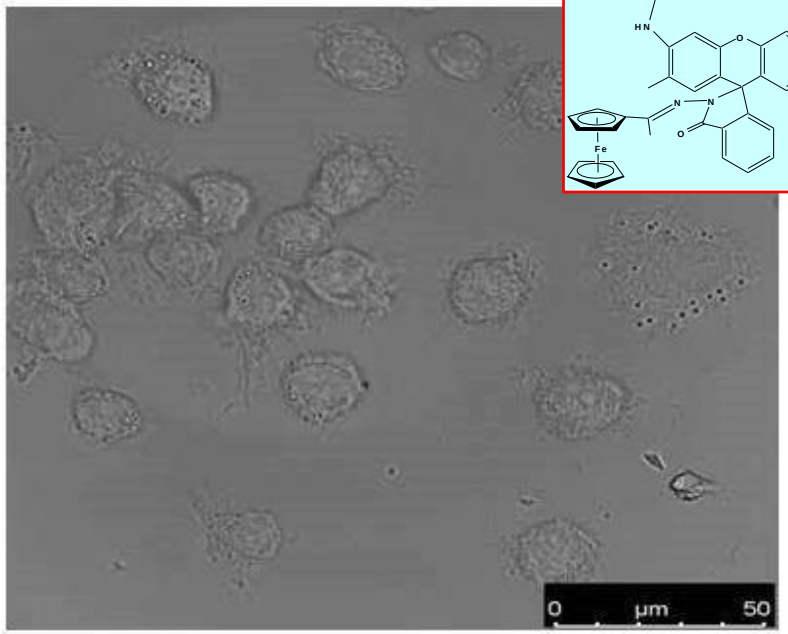

HN
NH
O
N
N
O
Fe

72 h

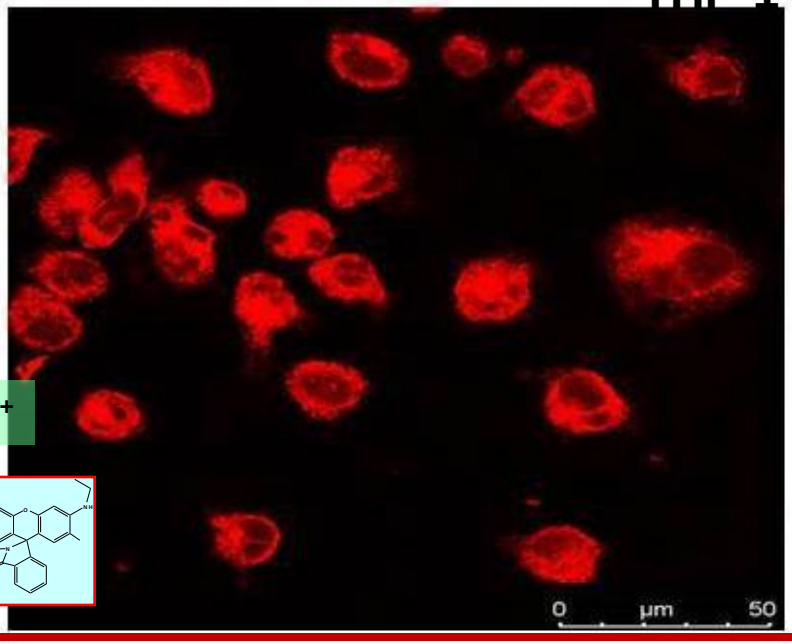

150
100
50
0
% viability
Control
DMSO
200 uM
100 uM
50 uM
25 uM
12.5 uM
MTT on THP -1 cell lines

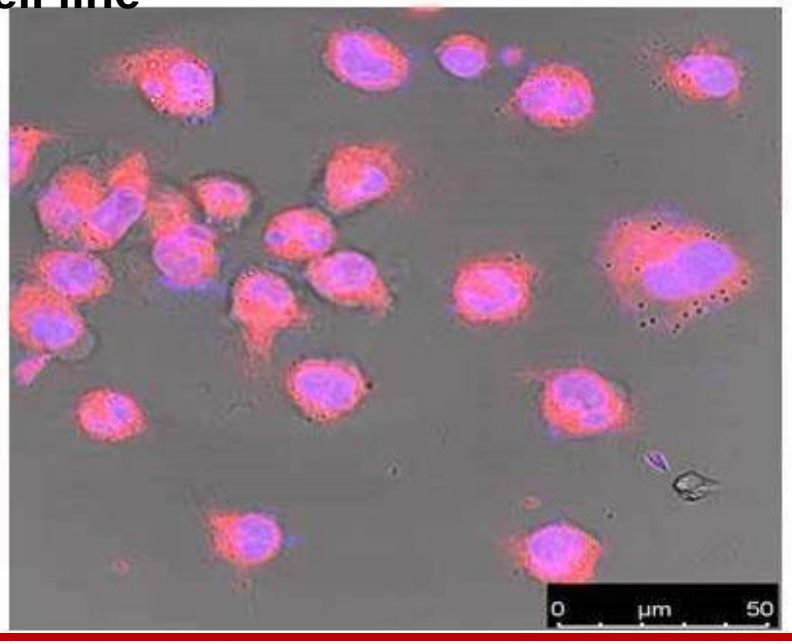


Nucleus staining

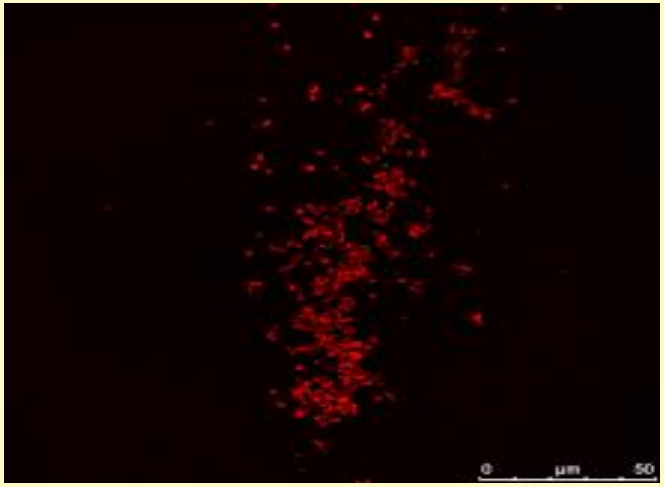


THP-1 cell line

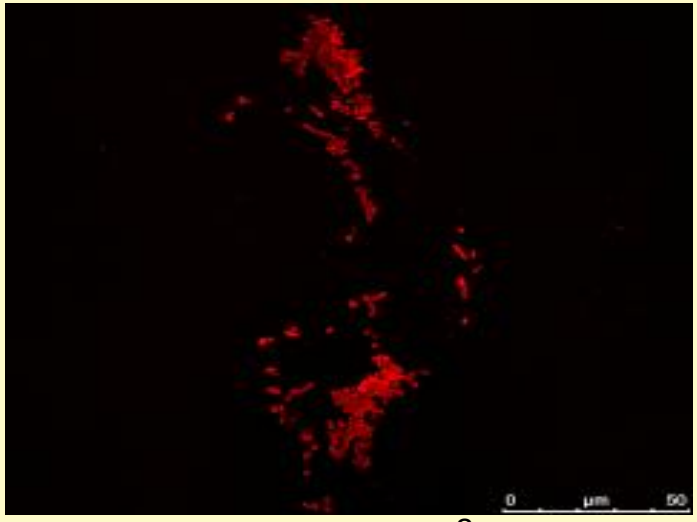




Hg^{2+}

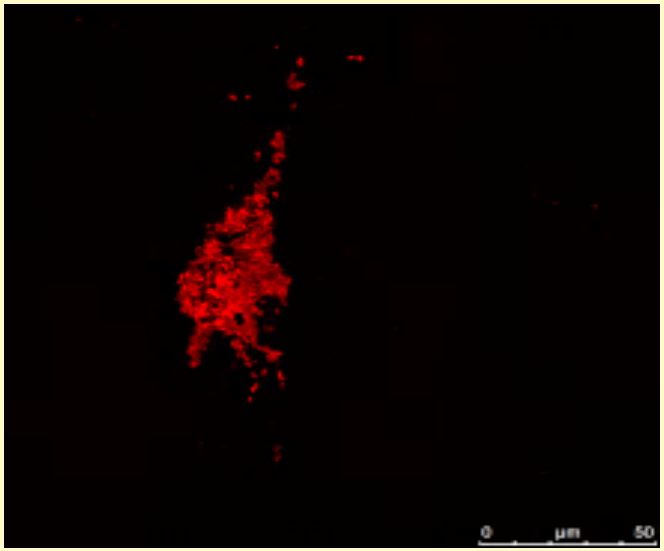


1 ppm Hg^{2+}

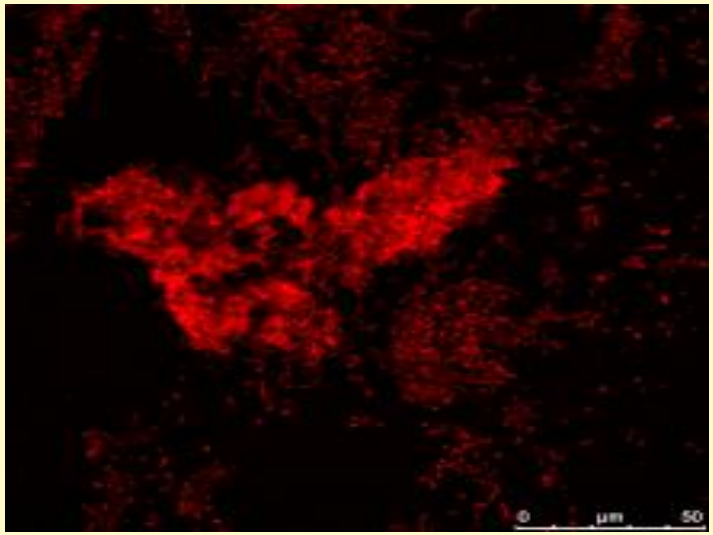


5 ppm Hg^{2+}

E. Coli

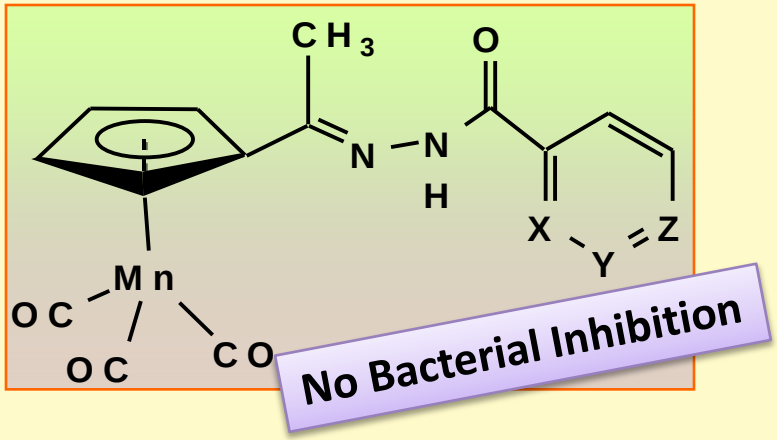


25 ppm Hg^{2+}

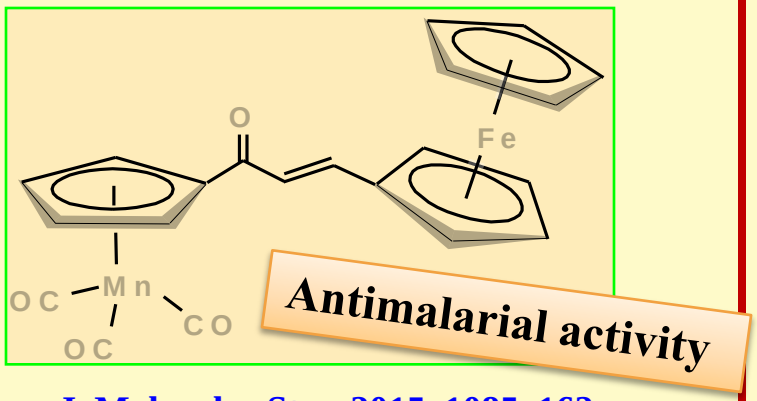


50 ppm Hg^{2+}

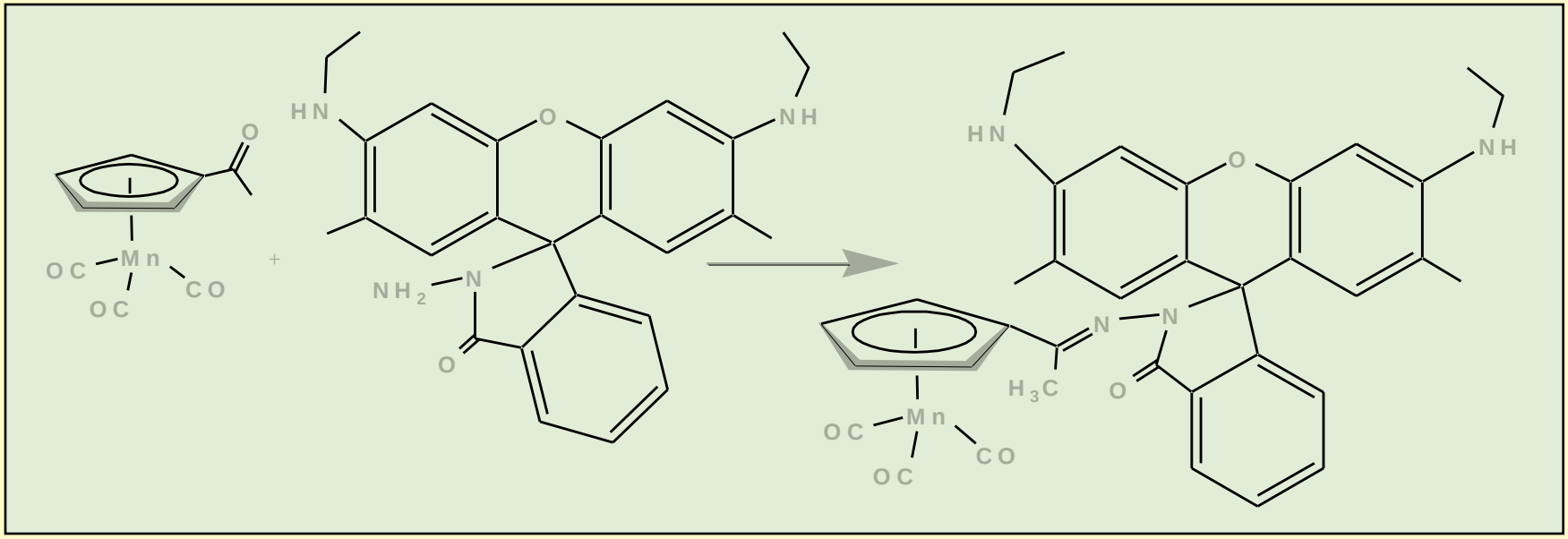
Half -Sandwich fluorescent hydrazone:

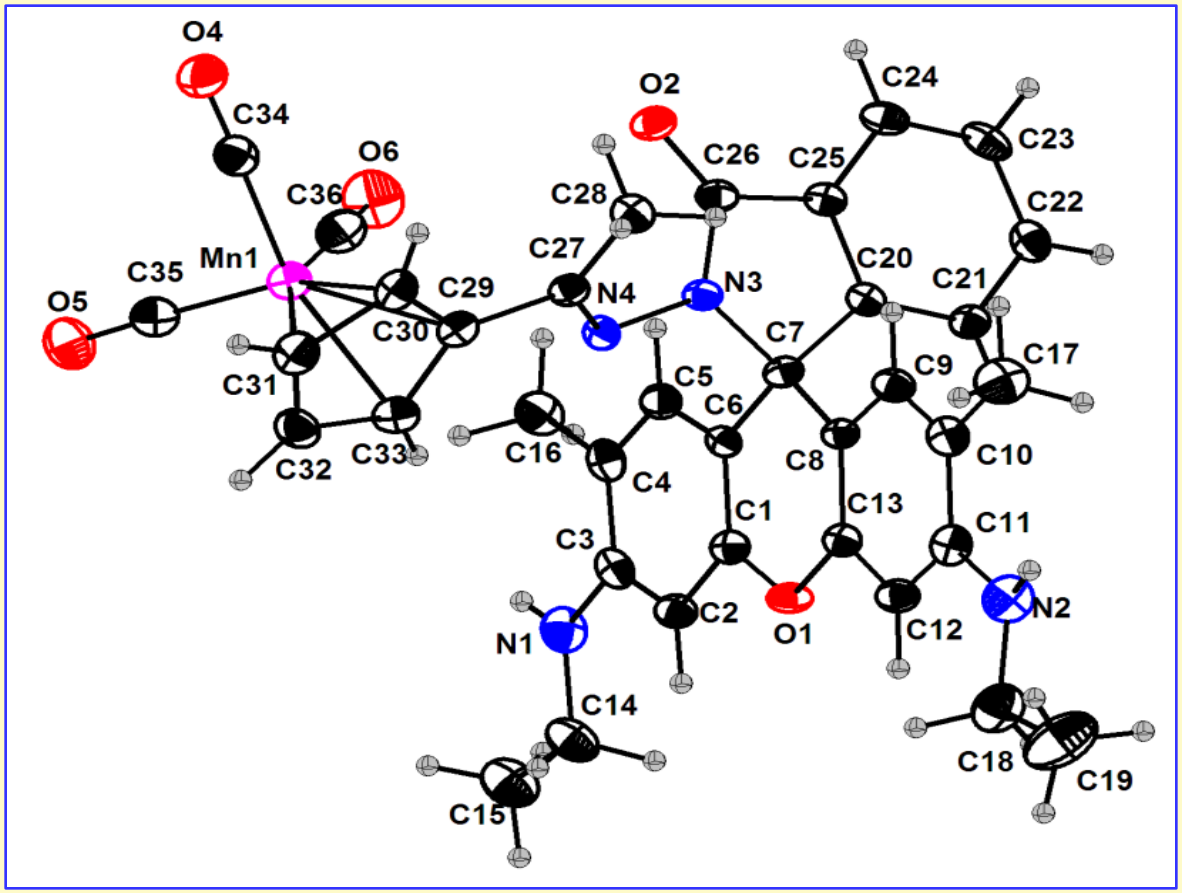


J. Organomet. Chem., 2013, *732*, 122



J. Molecular Str. , 2015, 1085, 162.





Triclinic, P -1

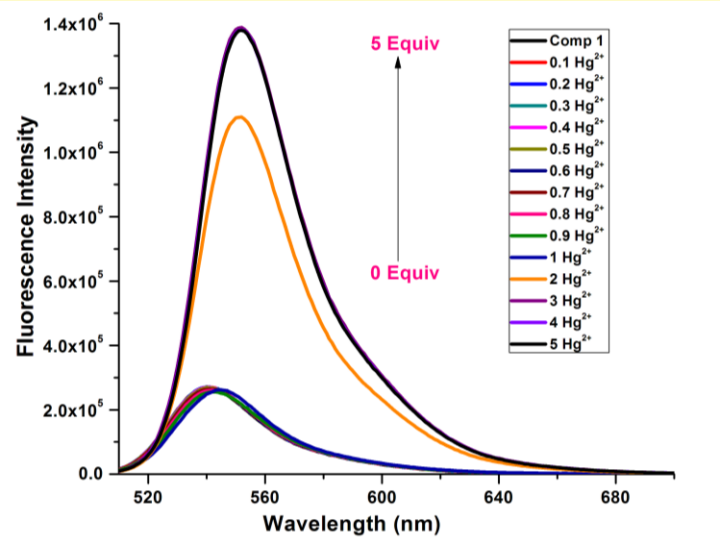
a= 9.5190(10) Å, b = 9.9598(9) Å, c = 17.3332(17) Å,

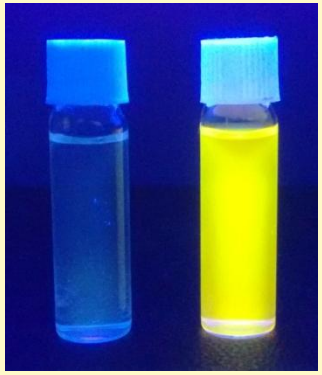
α=105.539(4)º, β =96.100(4)º,

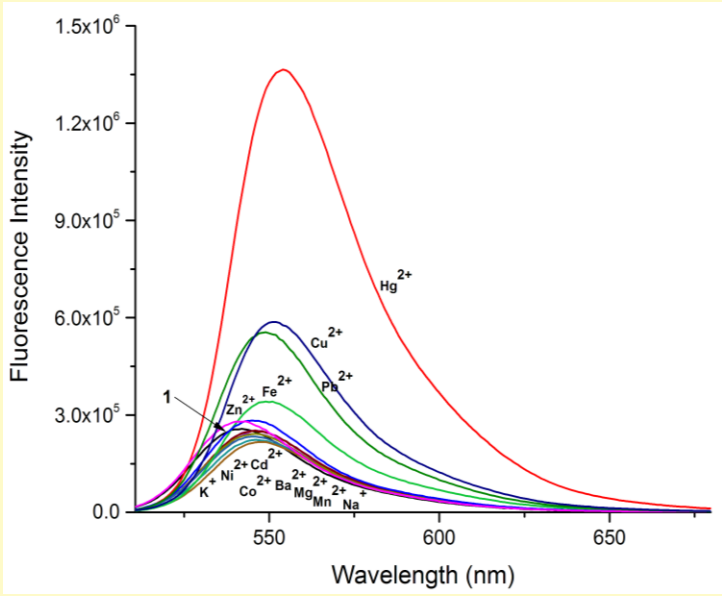
γ =96.788(4)º

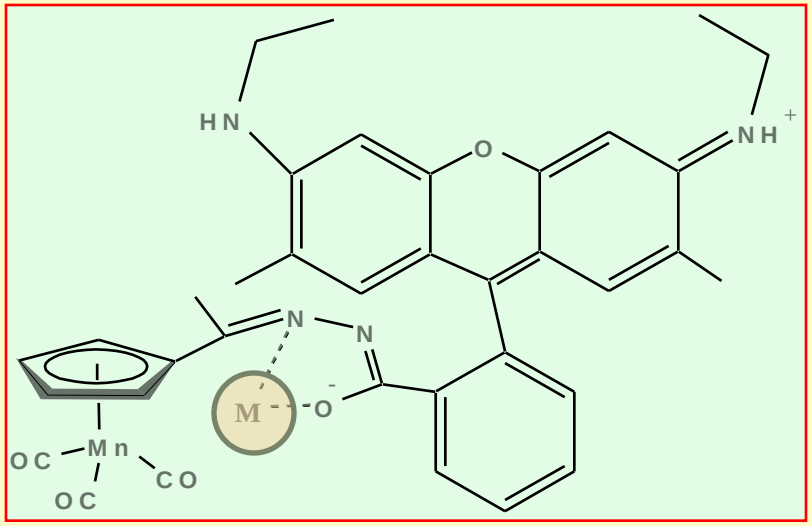
Selected bond lengths(Å) and bond angles(º): C(34)-O(4)= 1.147(4)Å, C(27)-N(4)=1.290(4)Å, N(4)-N(3)= 1.391(3)Å, N(3)-C(7)=1.495(4)Å, Mn(1)-C(35)=1.789(4)Å, C(26)-O(2)=1.219(4)Å, C(26)-N(3)-N(4)=124.7(2)º, C(25)-C(20)-C(7)=110.6(3)º, C(13)-O(1)-C(1)=118.2(2)º, C(27)-N(4)-N(3)=115.8(3)º

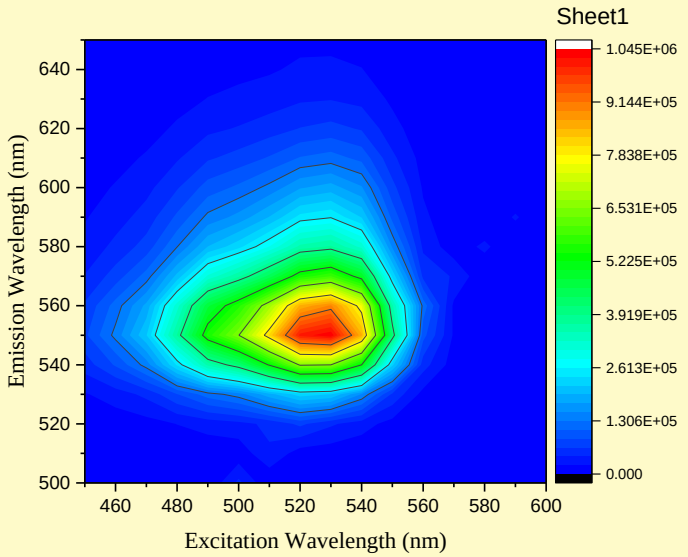
Selective Metal Sensing behavior:







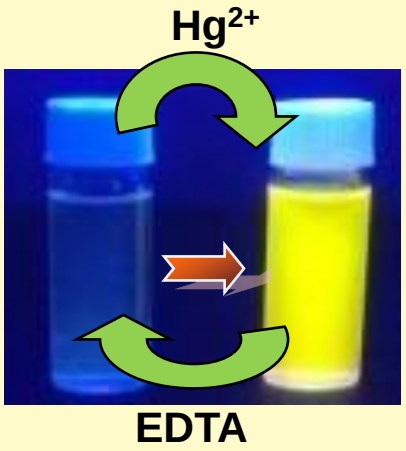




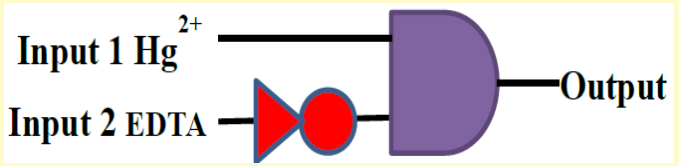
Communicated

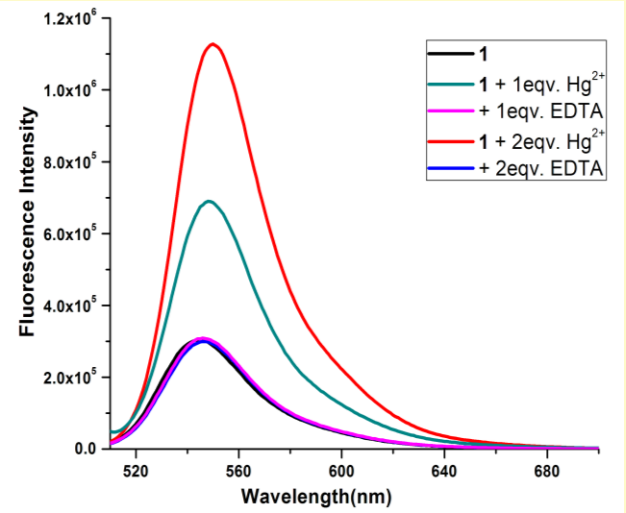
EEM Graph

“ON-OFF” molecular switch behavior



Circuit for INHIBIT logic gate





Truth Table: INHIBIT GATE

In (1) Hg^{2+}	*In (2) EDTA*	OUT (Fl Emission), λ_{em}=540
0	0	0
1	0	1
0	1	0
1	1	0

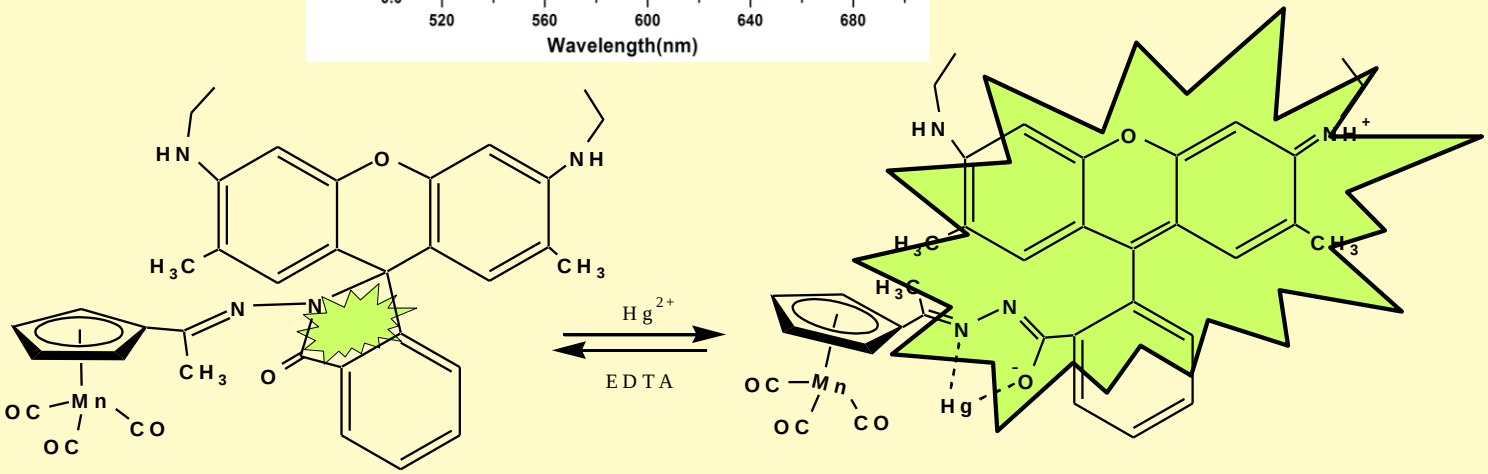
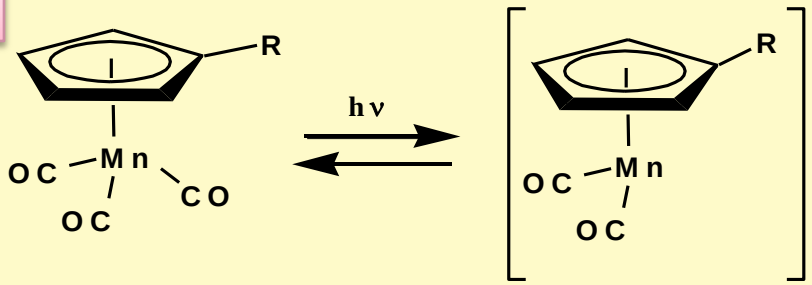
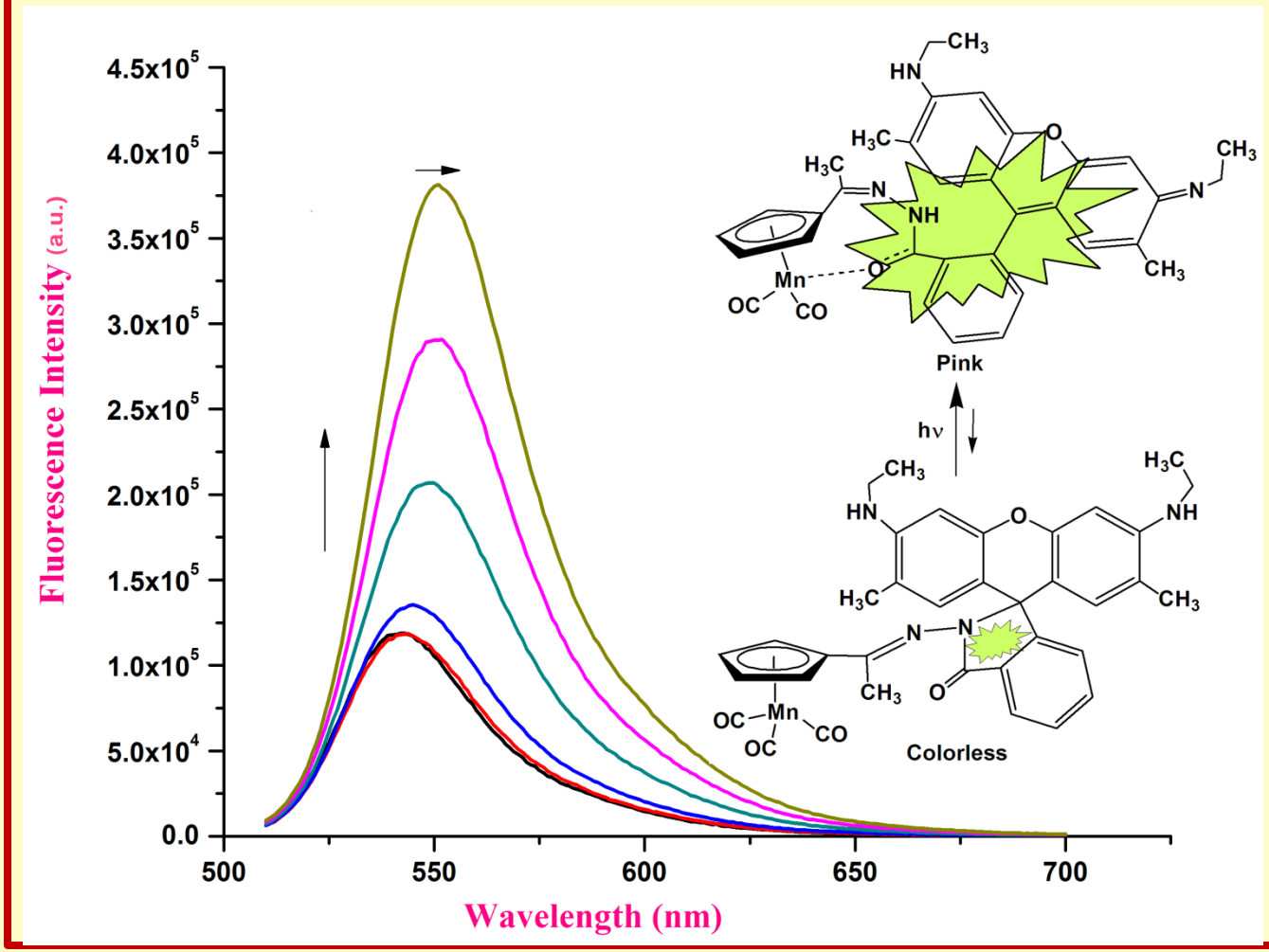
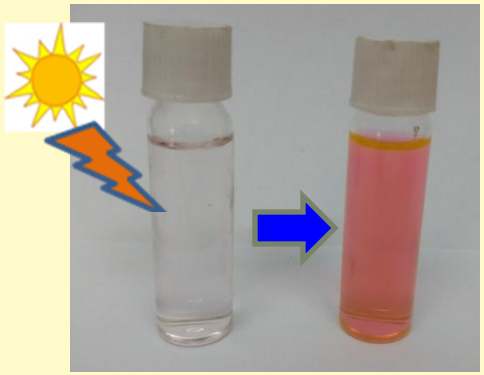


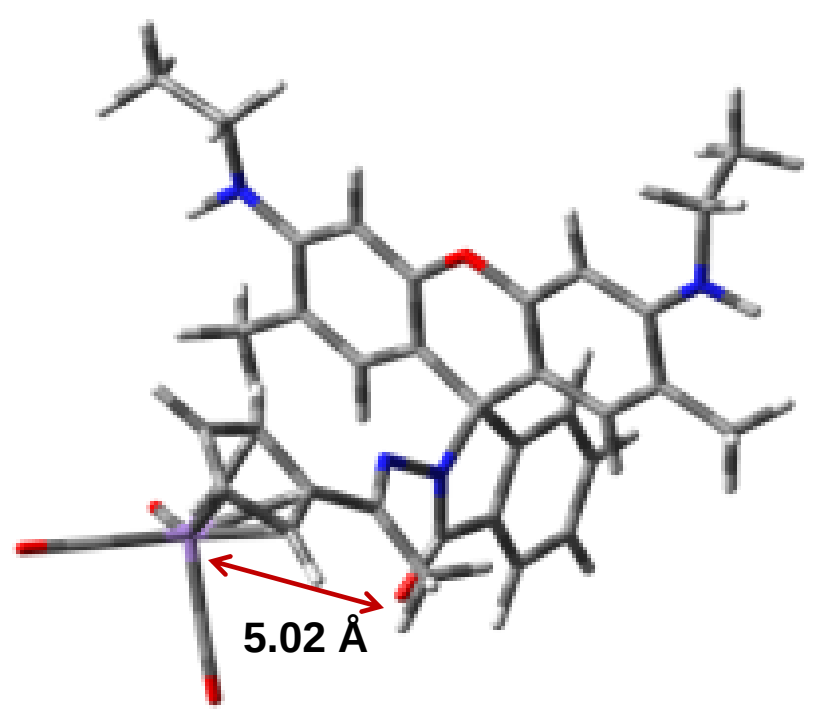
Photo-Responsive Behavior :

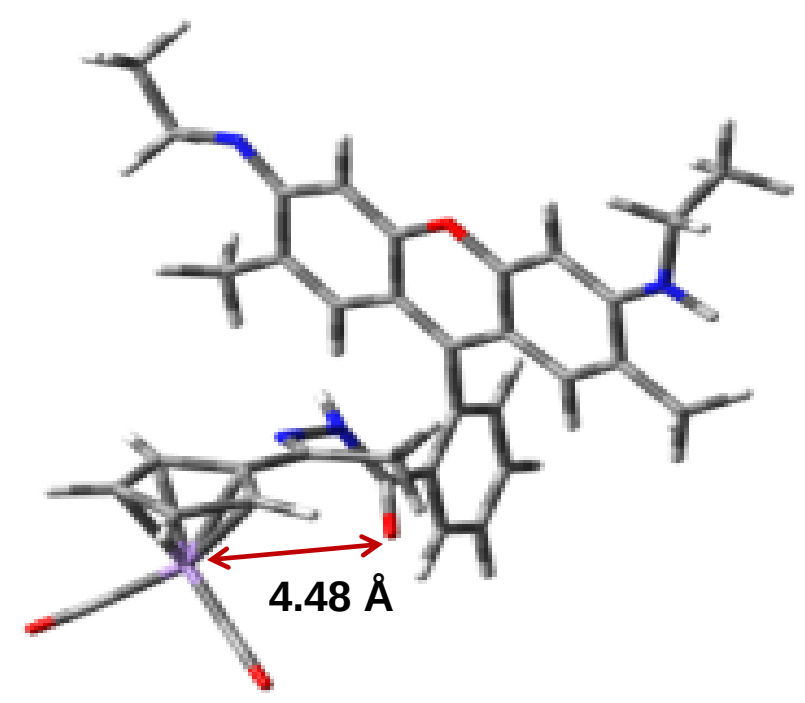




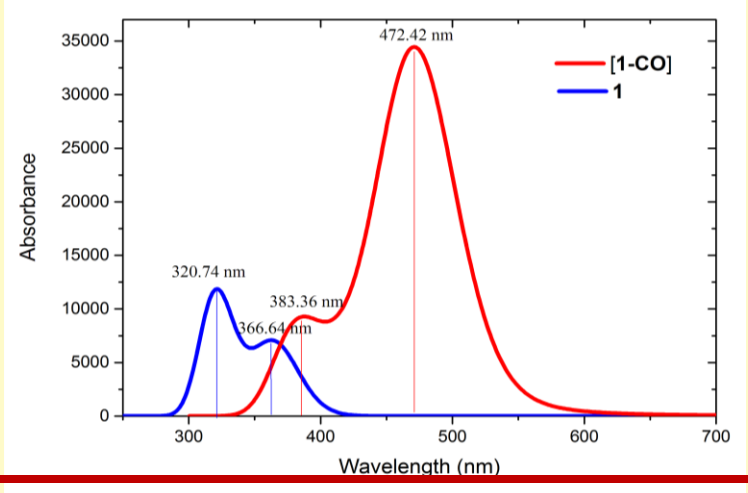


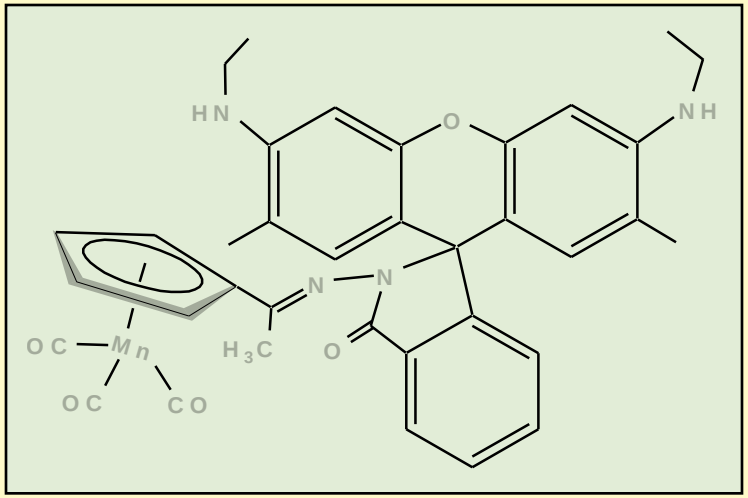
DFT-TDDFT Study:

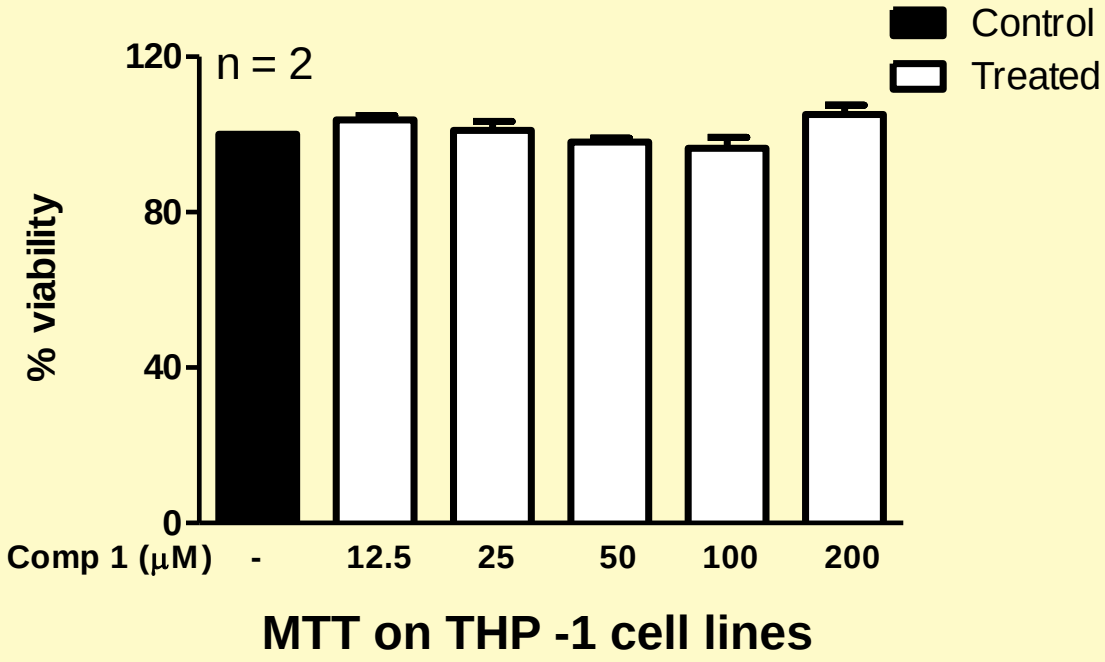


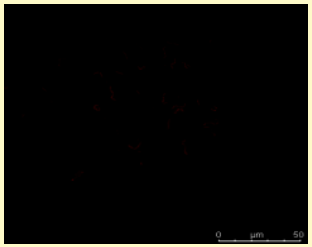


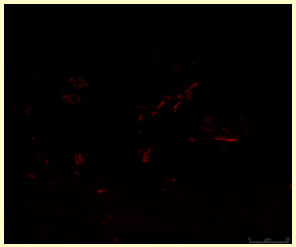
1 and [**1-CO**]

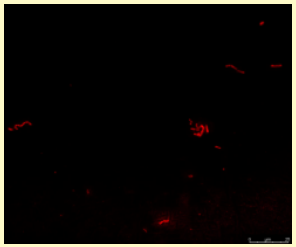



HN
O
NH
N
N
O C
Mn
H3C
O
O C
C O


Control
Treated
n = 2
120
80
40
0
% viability
Comp 1 (μM)
-
12.5
25
50
100
200
MTT on THP -1 cell lines


CpMnRhd


0.1 PPM Hg^{2+}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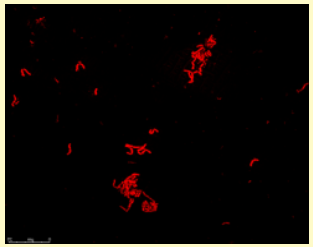
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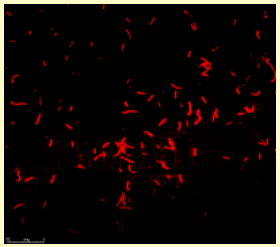
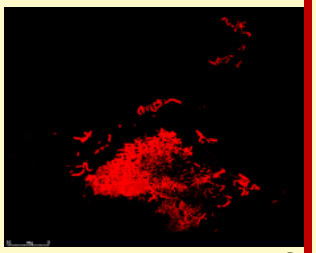
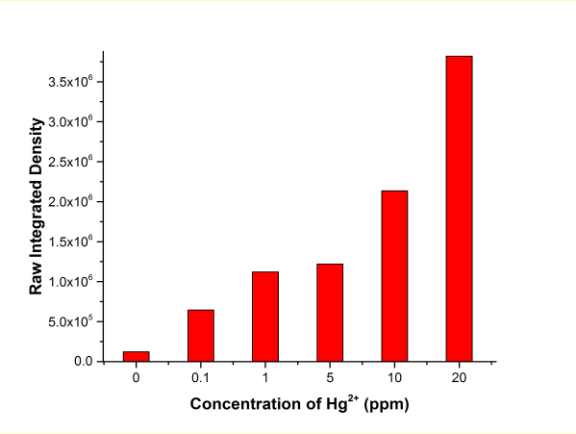

10 PPM Hg^{2+}

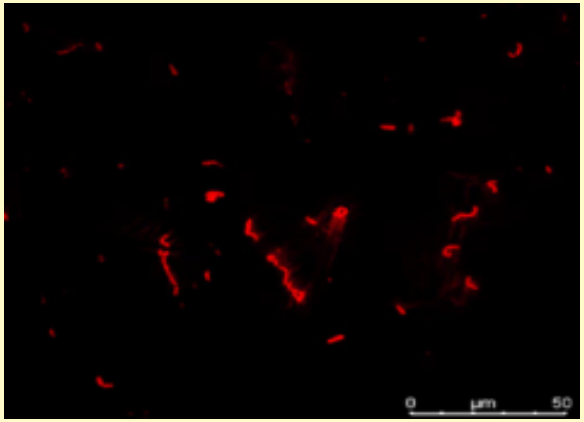

20 PPM Hg^{2+}

Fluorescence imaging in Bacterial cell *(P. aeruginosa)*

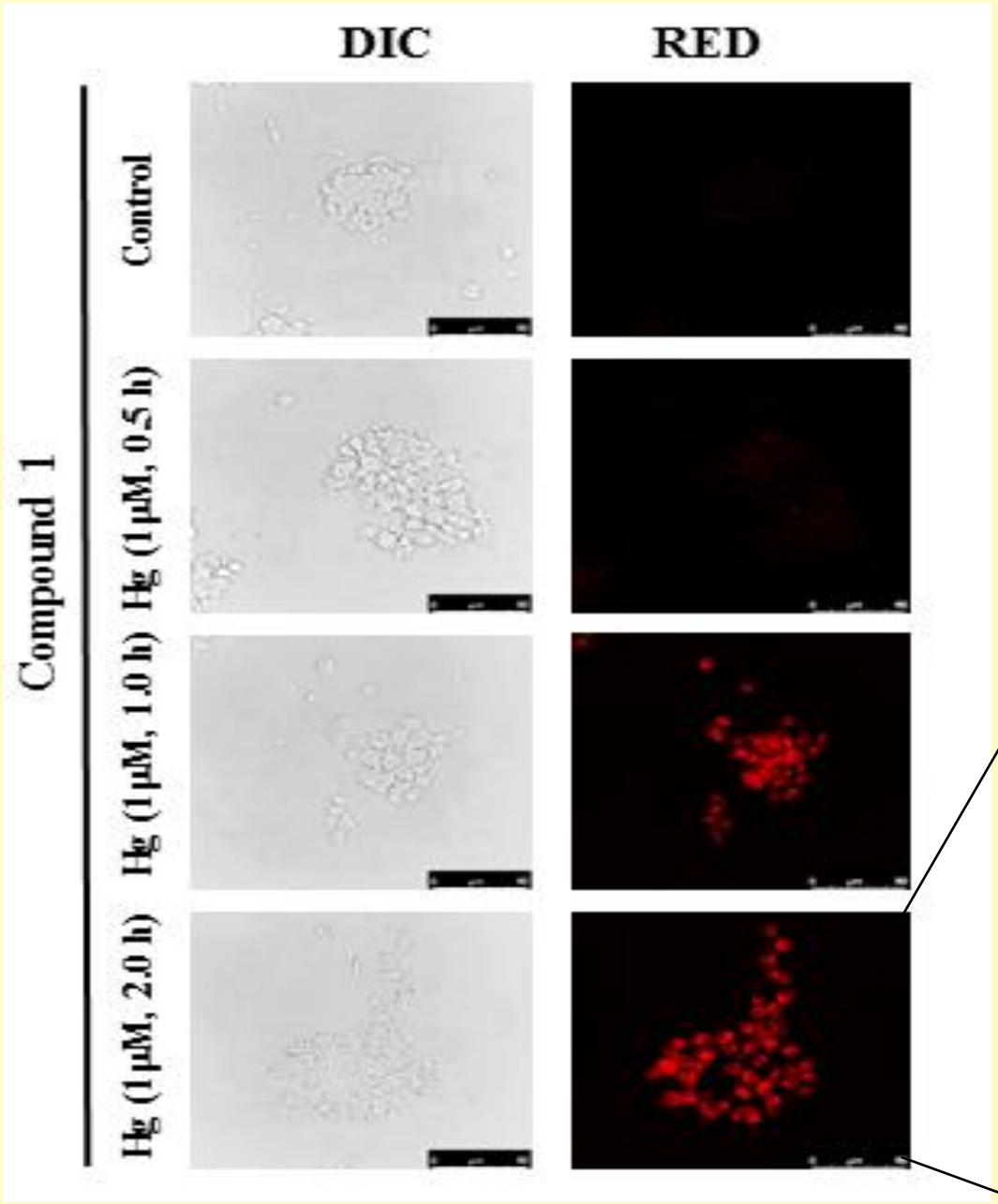


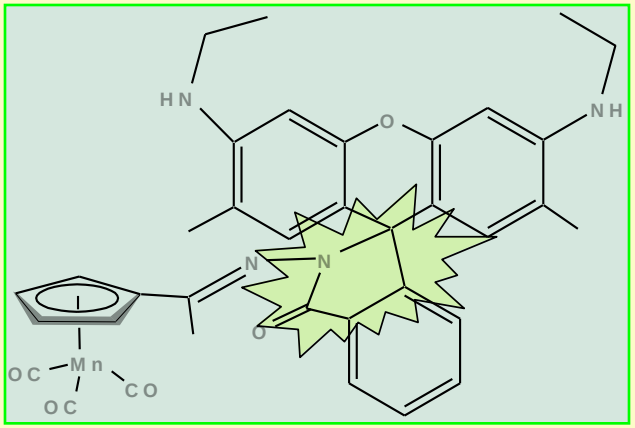
Light triggered CORM study is under progress

CpMnRhd + *P. aeruginosa*

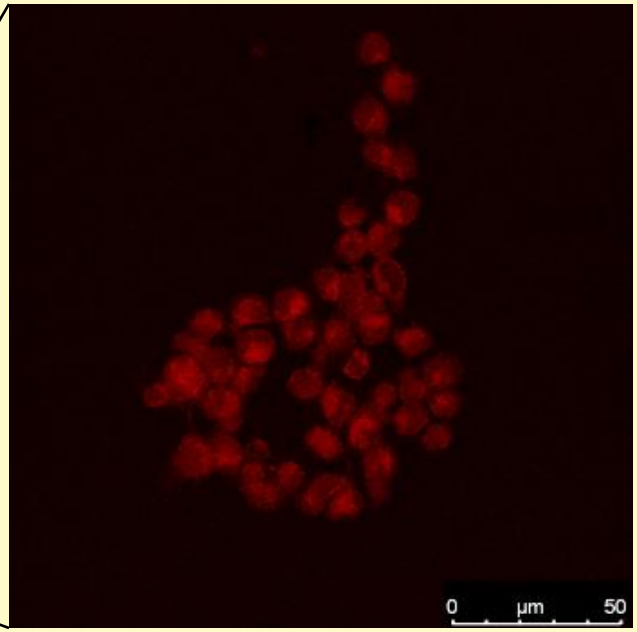


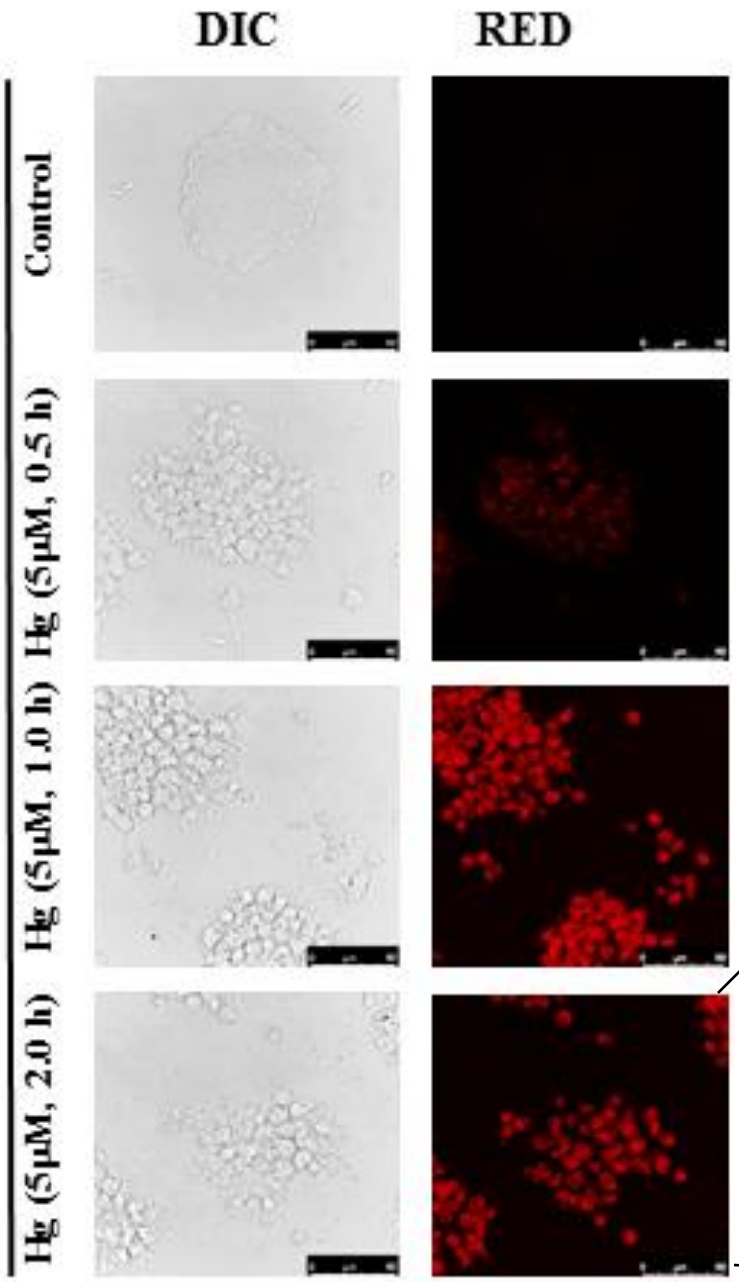
Under revision

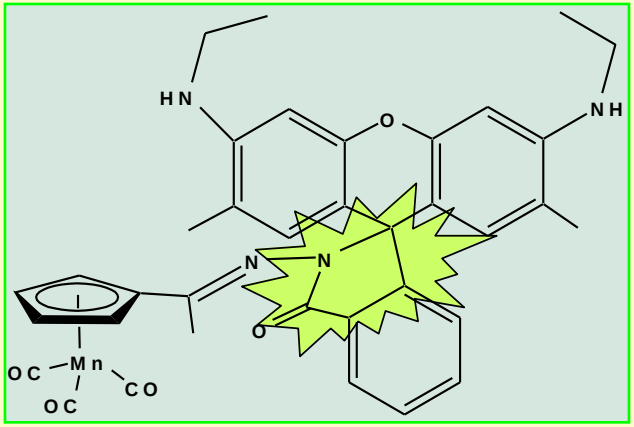




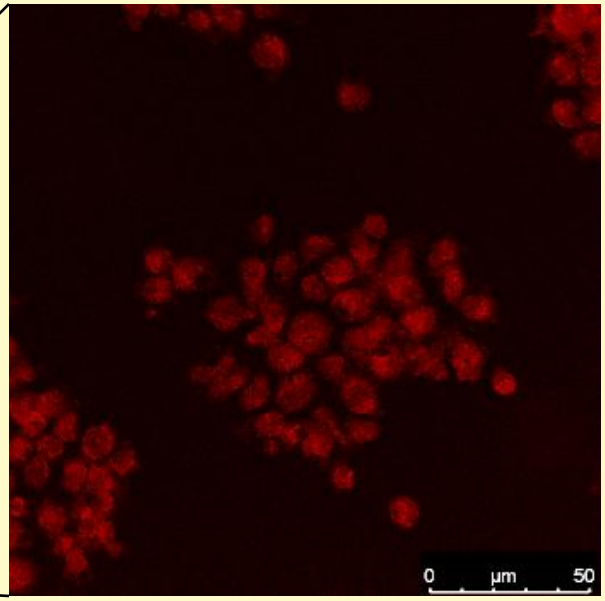
THP-1 cell line

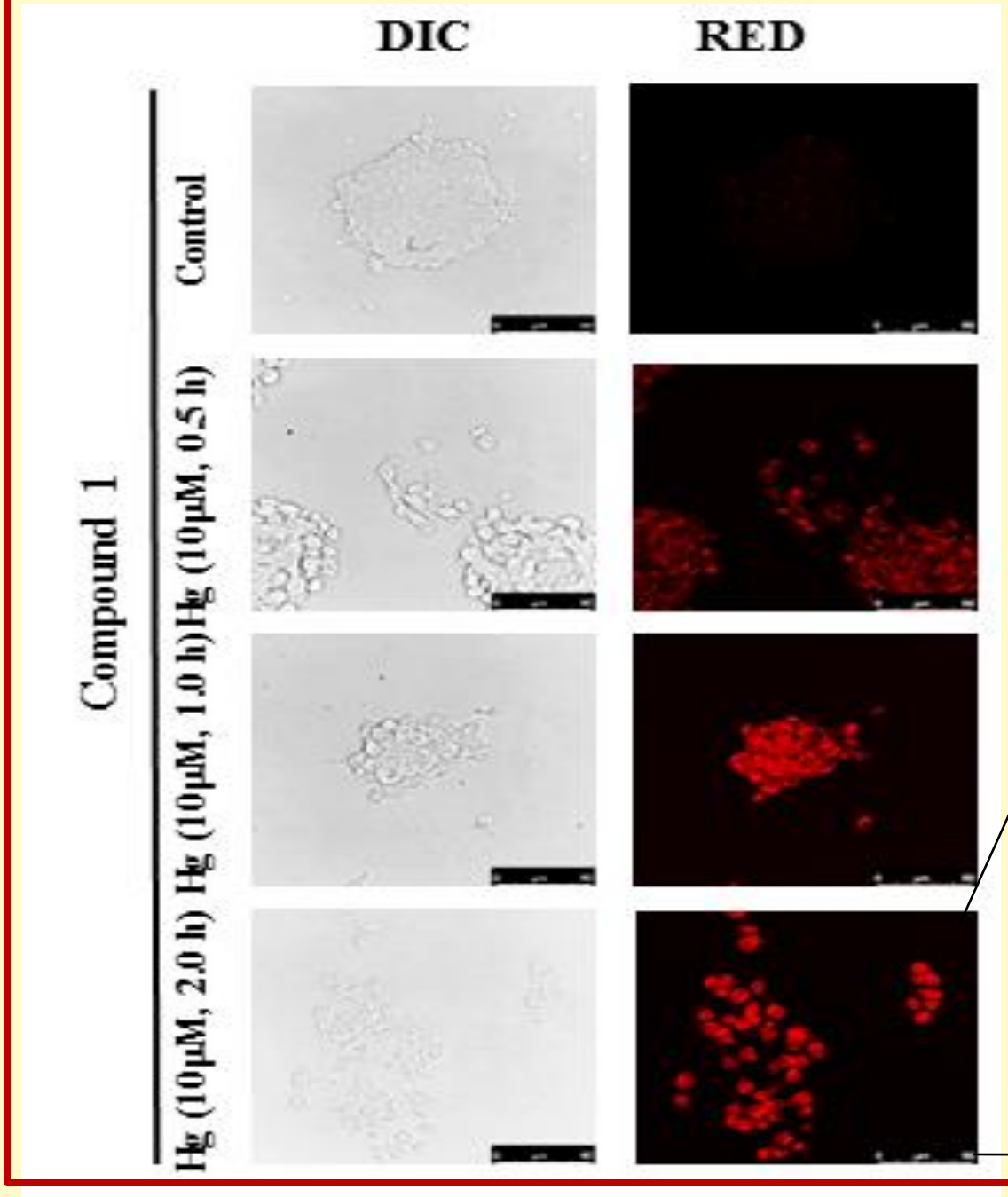


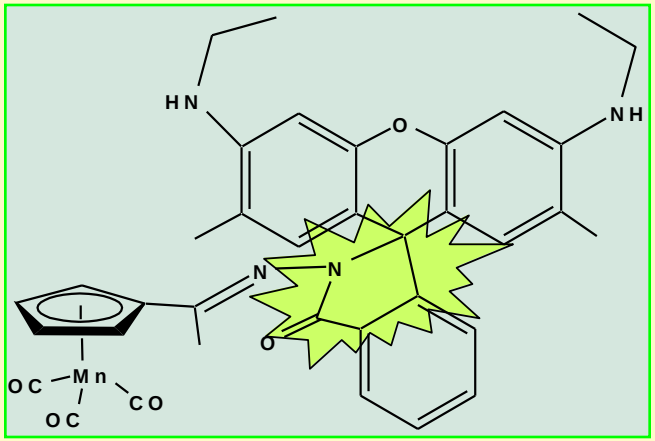




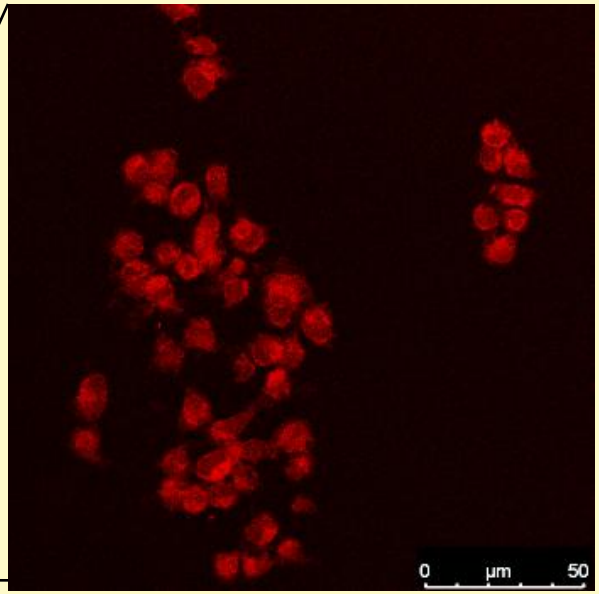
THP-1 cell line

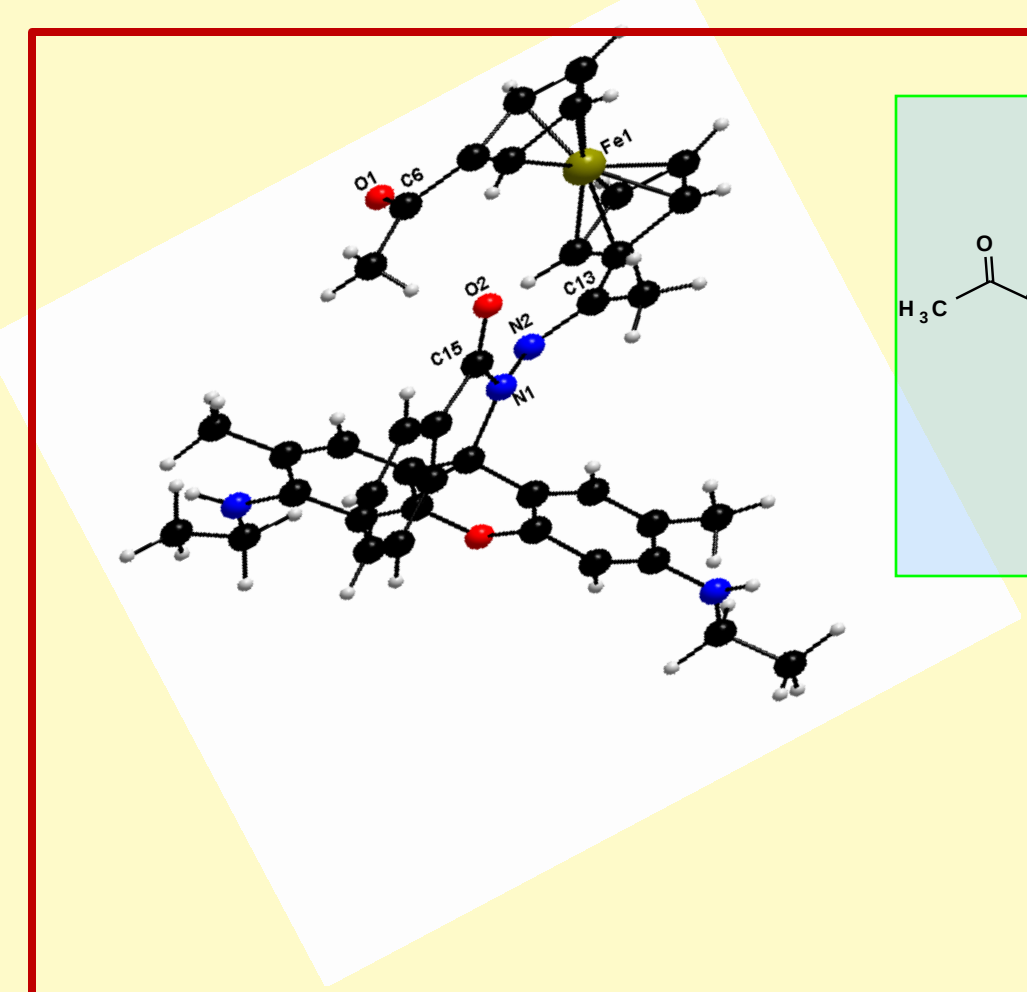


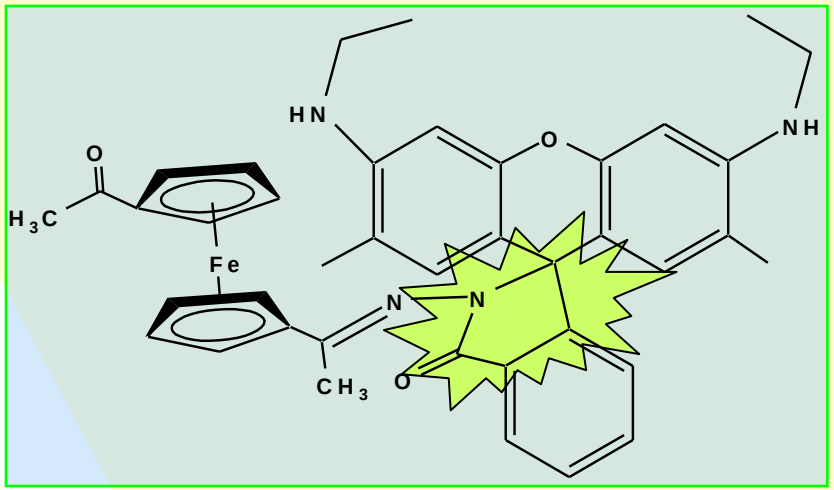


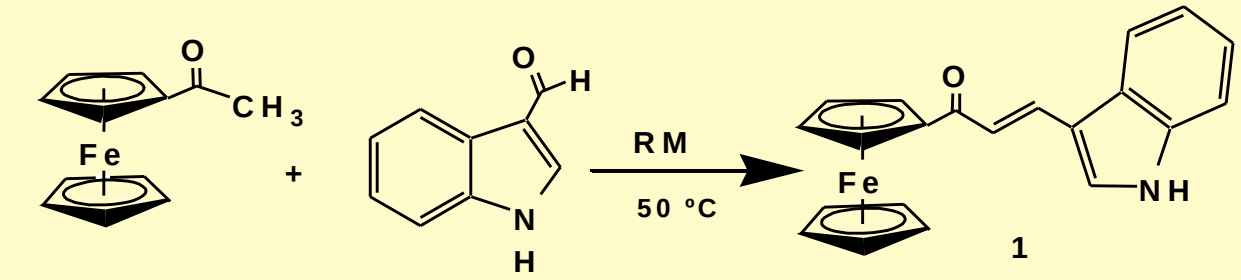


THP-1 cell line




Fe1
O1
C6
O2
C13
N2
C15
N1


HN
NH
O
O
H3C
Fe
N
N
CH3
O



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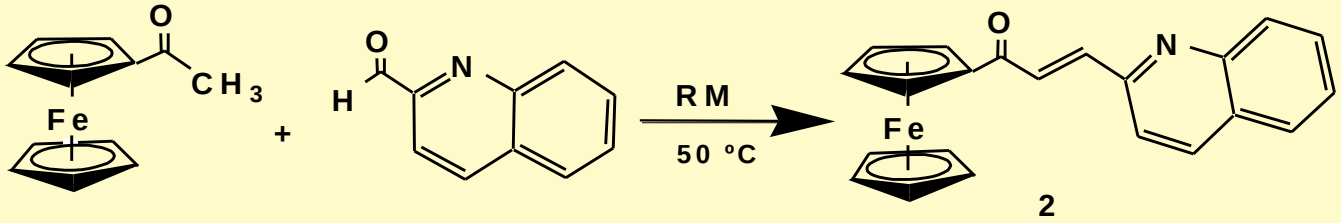

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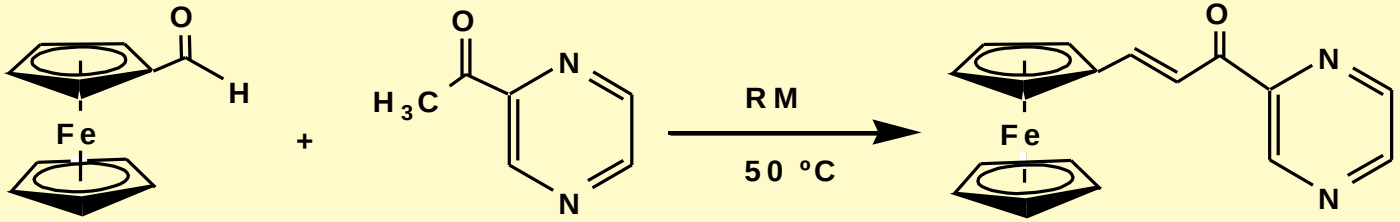

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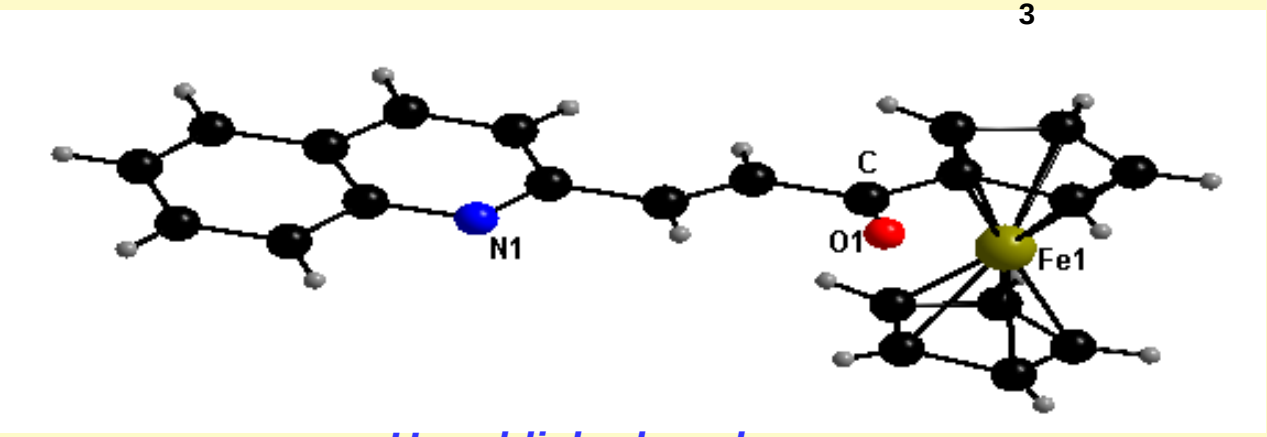
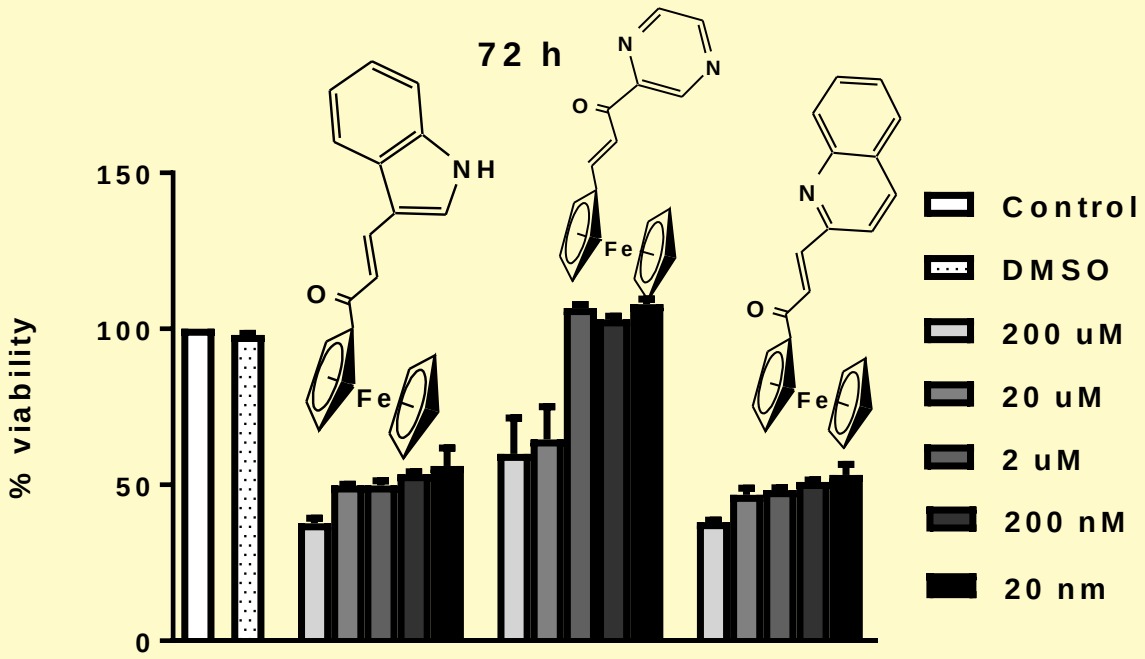
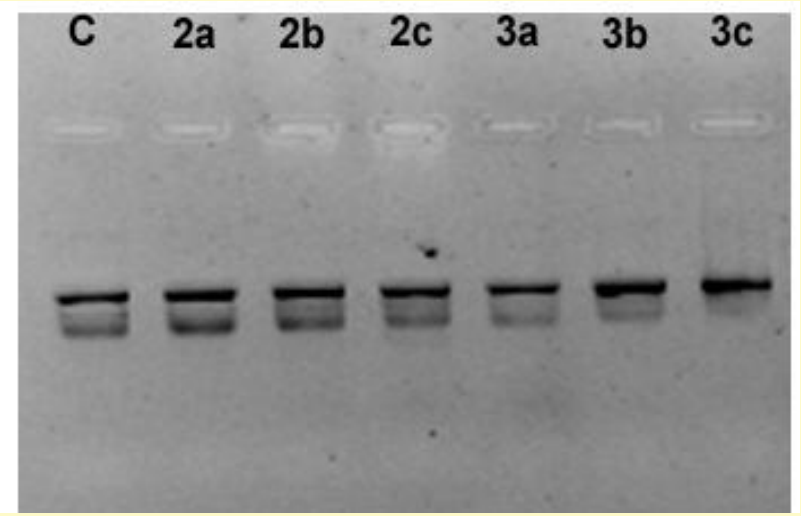
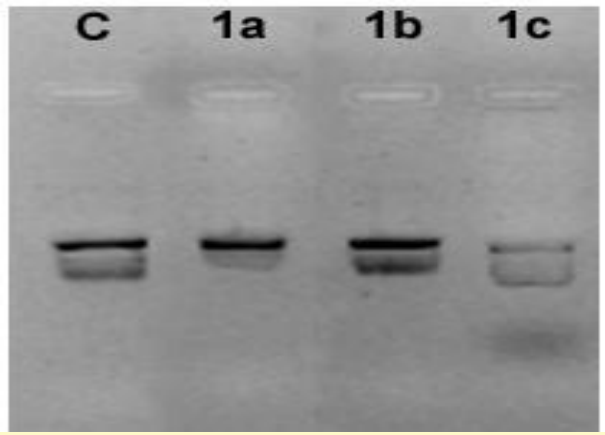


Unpublished work

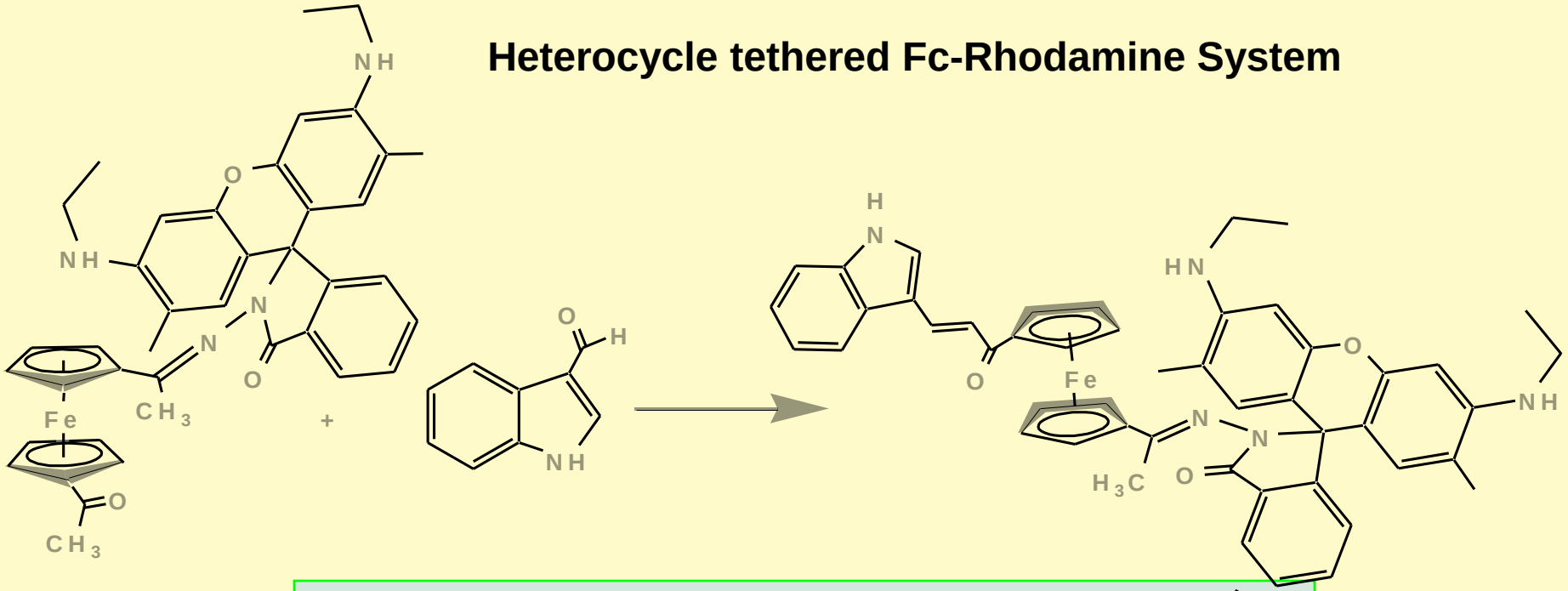


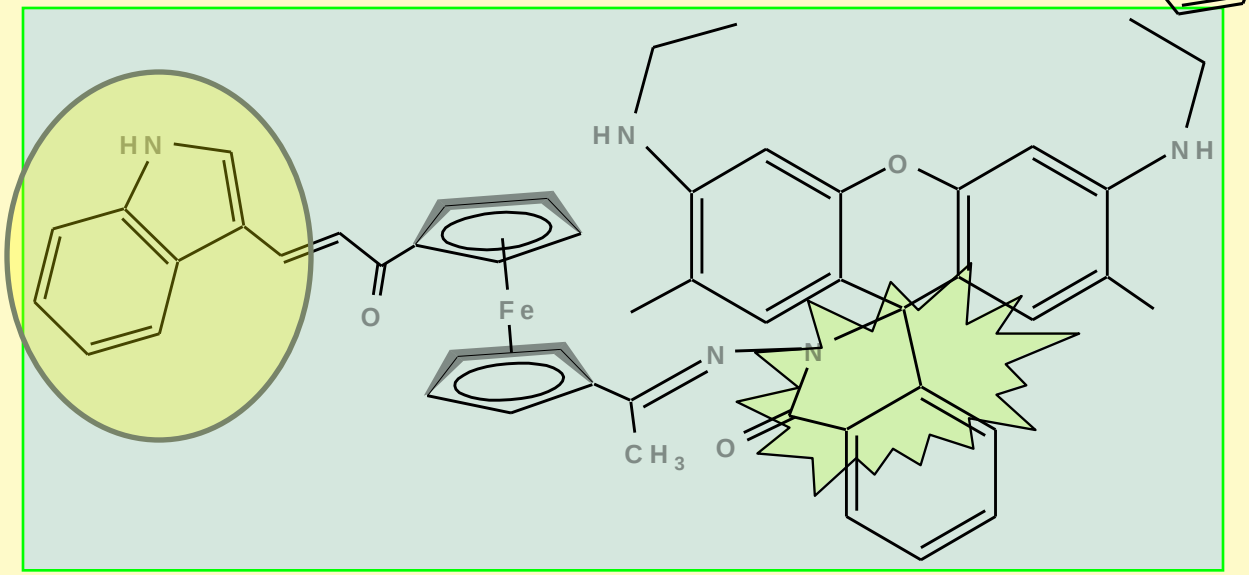




DNA Cleavage

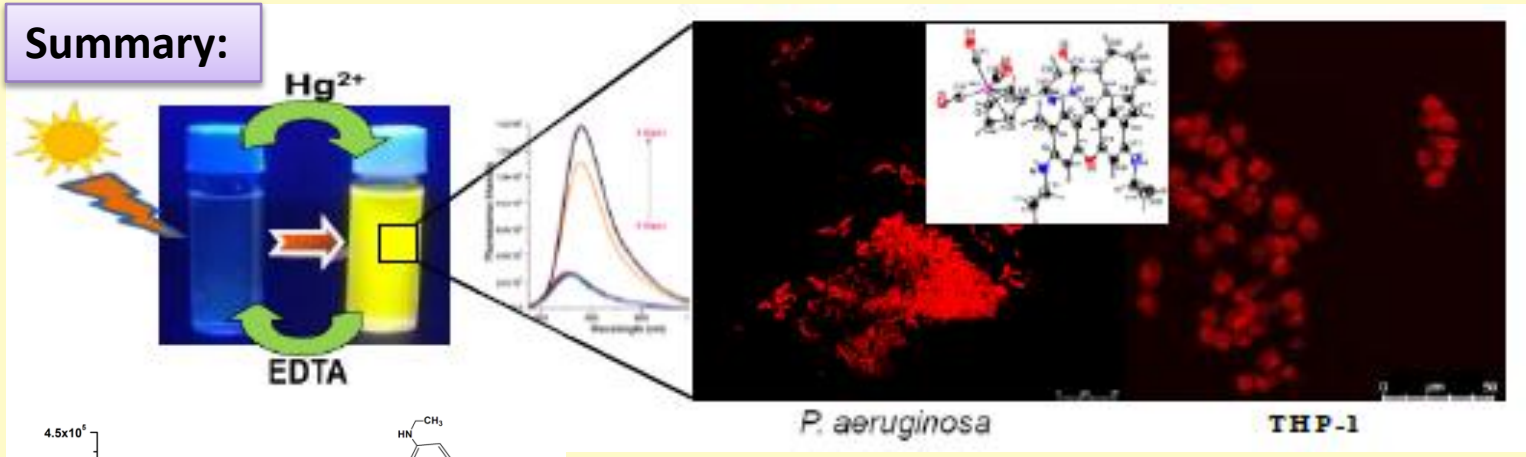
Heterocycle tethered Fc-Rhodamine System

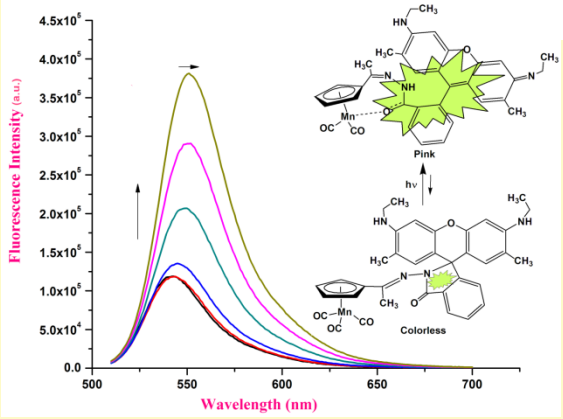


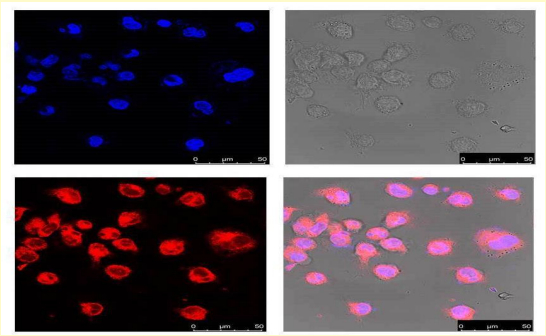


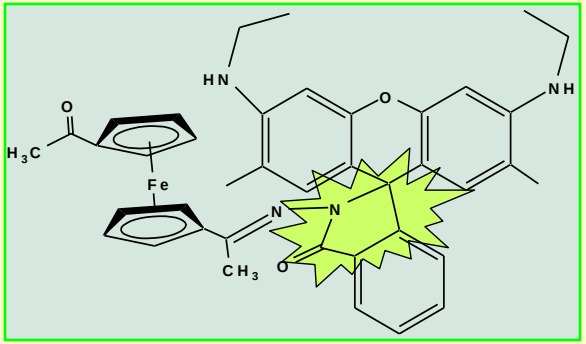
Under study

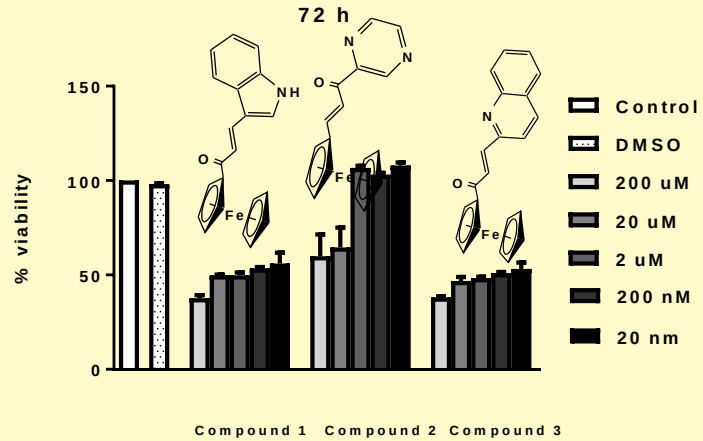
Summary:

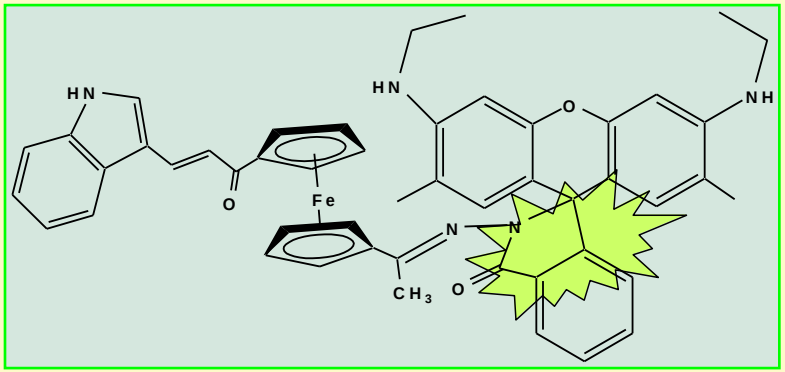

Hg2+
EDTA
P. aeruginosa
THP-1


Fluorescence Intensity (a.u.)
Wavelength (nm)
Pink
Colorless
hv






72 h
% viability
Control
DMSO
200 uM
20 uM
2 uM
200 nM
20 nm
Compound 1
Compound 2
Compound 3



Acknowledgements

Department of Science & Technology (SERB), India

Dr. S. M. Mobin, IIT Indore, India

Dr. C. Wölper, Uni Duisburg-Essen, Germany

Dr. S. Das & Dr. R. Dhiman, Dept. of Life Science, NIT Rourkela,

Dr. Santanab Giri, Theoretical Chemistry Lab, NIT Rourkela

Compliments to my brigade


THANK YOU