Synthesis of $\eta^5$-C$_5$H$_4$R based compounds with functional moieties for sensing and imaging applications.

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Ferrocenyl based system

Sandwich

Ferrocenyl – heterocycle system

Half Sandwich

Cymantrenyl– heterocycle system

Bifunctional Diferrocenyl system

Ferrocenyl – Half sandwich based

Ferrocene based Multimetallic clusters
Selectively binds Pb$^{2+}$ cation

Selective Functionalization:

\[
\text{CH}_3\text{C} = \text{N} - \text{N} - \text{C} - \text{OH} ; \text{Y} = \text{CH}, \text{N} ; \\
\text{Z} = \text{CH}, \text{N}
\]

High antibacterial activity!!

Rice Husk Silica

Only product
\[
\text{Vac} \quad \text{NaOH} \\
\begin{align*}
X &= Y = Z = \text{CH} \\
X &= \text{C-OH}, \quad Y = Z = \text{CH} \\
X &= Z = \text{CH}, \quad Y = \text{N} \\
X &= Y = \text{CH}, \quad Z = \text{N}
\end{align*}
\]
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.

Metal ions are essential for Microorganisms during the process of infection and are involved in bacterial metabolism and various virulence 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:

\[
\text{Sandwich fluorescent hydrazone:}
\]

Zn\(^{2+}\) and Cd\(^{2+}\) also showed interaction
Redox Switch:

![Graph showing fluorescence intensity vs. wavelength](image-url)

![Chemical structure diagram](image-url)
MTT on THP-1 cell lines

% viability

72 h

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+}
Half-Sandwich fluorescent hydrazone:


J. Molecular Str. , 2015, 1085, 162.
Triclinic, P -1

\[ a = 9.5190(10) \text{ Å}, \ b = 9.9598(9) \text{ Å}, \ c = 17.3332(17) \text{ Å},\]
\[ \alpha = 105.539(4) ^\circ, \ \beta = 96.100(4) ^\circ, \ \gamma = 96.788(4) ^\circ \]

Selected bond lengths (Å) and bond angles (°):
- 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) °,
- C(25)-C(20)-C(7) = 110.6(3) °, C(13)-O(1)-C(1) = 118.2(2) °,
- C(27)-N(4)-N(3) = 115.8(3) °
Selective Metal Sensing behavior:

Communicated
“ON-OFF” molecular switch behavior

Circuit for INHIBIT logic gate

Input 1 Hg$^{2+}$
Input 2 EDTA

Output

Truth Table: INHIBIT GATE

<table>
<thead>
<tr>
<th>In (1) Hg$^{2+}$</th>
<th>In (2) EDTA</th>
<th>OUT (Fl Emission), $\lambda_{em}$=540</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
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<td>0</td>
</tr>
<tr>
<td>1</td>
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<tr>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

Fluorescence intensity vs. Wavelength (nm)

[molecular structures and graphs]

Circuit for INHIBIT logic gate

Hg$^{2+}$
EDTA

“ON-OFF” molecular switch behavior
Photo-Responsive Behavior:

\[
\begin{align*}
&\text{OC} \quad \text{Mn} \quad \text{CO} \\
&\text{OC} \quad \text{Mn} \quad \text{OC} \\
&\text{OC} \quad \text{Mn} \quad \text{CO}
\end{align*}
\]

\[\text{hv} \rightarrow \]

\[
\begin{align*}
&\text{OC} \quad \text{Mn} \quad \text{CO} \\
&\text{OC} \quad \text{Mn} \quad \text{OC} \\
&\text{OC} \quad \text{Mn} \quad \text{CO}
\end{align*}
\]

Fluorescence Intensity (a.u.)

Wavelength (nm)
DFT-TDDFT Study:

1 and [1-CO]

5.02 Å

4.48 Å
Comp 1 (μM) - 12.5 25 50 100 200
Control
Treated

n = 2

% viability

MTT on THP-1 cell lines

Comp 1 (μM) - 12.5 25 50 100 200
Control
Treated

n = 2
Fluorescence imaging in Bacterial cell (*P. aeruginosa*)

Light triggered CORM study is under progress

CpMnRhd + *P. aeruginosa*
Compound 1

<table>
<thead>
<tr>
<th></th>
<th>DIC</th>
<th>RED</th>
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</thead>
<tbody>
<tr>
<td>Control</td>
<td><img src="image1" alt="DIC" /></td>
<td><img src="image2" alt="RED" /></td>
</tr>
<tr>
<td>Hg (1µM, 0.5 h)</td>
<td><img src="image3" alt="DIC" /></td>
<td><img src="image4" alt="RED" /></td>
</tr>
<tr>
<td>Hg (1µM, 1.0 h)</td>
<td><img src="image5" alt="DIC" /></td>
<td><img src="image6" alt="RED" /></td>
</tr>
<tr>
<td>Hg (1µM, 2.0 h)</td>
<td><img src="image7" alt="DIC" /></td>
<td><img src="image8" alt="RED" /></td>
</tr>
</tbody>
</table>

THP-1 cell line
THP-1 cell line
Unpublished work
DNA Cleavage

% viability

C O m p o u n d  1  C o m p o u n d  2  C o m p o u n d  3

C o n t r o l  D M S O  2 0 0  u M  2 0  u M  2  u M  2 0 0  n M  2 0  n m

F e  O  N  H

C o m p o u n d  1  C o m p o u n d  2  C o m p o u n d  3

% viability

C o n t r o l  D M S O  2 0 0  u M  2 0  u M  2  u M  2 0 0  n M  2 0  n m

C o m p o u n d  1  C o m p o u n d  2  C o m p o u n d  3

D N A  C l e a v a g e
Heterocycle tethered Fc-Rhodamine System

Under study
Summary:

[Diagram showing chemical structures and graphs related to viability studies.]
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Compliments to my brigade
THANK YOU