Synthesis, Characterization and Biological Studies of Trinuclear Nd(III) Salen Capped Complex with 2,4,6-tris(4-carboxybenzimino)-1,3,5-triazine

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ABSTRACT

A novel trinuclear Nd(III) salen capped complex of 2,4,6-tris(4-carboxybenzimino)-1,3,5-triazine was synthesized for the first time by the reaction of Nd(III) ligand complex with 2,4,6-tris(4-carboxybenzimino)-1,3,5-triazine. The ligand and complex were characterized using UV-Visible, IR, ¹H and ¹³C NMR spectroscopies, elemental analysis, and molar conductivity measurements. The spectral studies indicate that the ligand is hexadentate and coordinates to Nd(III) ions through the oxygen atoms of the carboxylic group. The trinuclear Nd(III) salen capped complex was characterized as being bridged by carboxylate anions to the Nd(III) salen centers and displays a coordination number of eight by involving two hydroxyl groups in the coordination sphere. The in vitro antimicrobial activities of the ligand and its Nd(III) salen capped complex were investigated against Gram-negative bacteria: Escherichia coli (ATCC 6749) and Pseudomonas aeruginosa (ATCC 9027), Gram-positive bacteria: Staphylococcus aureus (ATCC 6538P) and Bacillus cereus (ATCC 14579), and fungi: Candida albicans and Aspergillus niger by the agar well diffusion technique. The ligand was found to be more potent against the test microorganisms relative to the trinuclear Nd(III) salen capped complex. The trinuclear Nd(III) salen capped complex inhibits the growth of Bacillus cereus, Staphylococcus aureus, Pseudomonas aeruginosa, Escherichia coli, Candida albicans, and Aspergillus niger at concentrations of 50 μg/mL.

(Keywords: synthesis, trinuclear Nd(III) salen capped complex, antimicrobial activity)

INTRODUCTION

The study of lanthanides and lanthanide compounds have aroused much interest because they have applications in medicinal inorganic chemistry and in material science (Salehzadeh et al., 2005). In medicine, lanthanide complexes are exploited as contrast agents for magnetic resonance imaging (MRI) and as radiotherapeutic drugs (Salehzadeh et al., 2005; Casellato et al., 1996). Due to the catalytic, magnetic, and luminescent properties of lanthanide complexes with organic ligands, they have found application in electroluminescent devices and diodes, lasers, cathode ray tubes, sensors, dosimeters, biological fluoro-immunoassays, imaging agent, organic light emitting diodes (OLEDs), display application, decoration purposes, and telecommunication (Mihalyova et al., 2014; Chen et al., 2015; Fei et al., 2016; Liu et al., 2013). Lanthanide complexes with desired functions have been designed and synthesized using different kinds of organic ligands (Chen et al., 2013; Yue et al., 2015).

Lanthanides complexes with various organic ligands exhibit a wide range of pharmacological properties such as anticancer (Dalla Cort et al., 2010), cytotoxic and cytostatic activities (Kostova et al., 2004, Kostova et al., 2005), antioxidant (Bashir and Abdulhadi, 2017), antibacterial (Lekha et al., 2014; Mohanan et al., 2014) and antitumor activity (Chen et al., 2013; Kostova et al., 2001). To the best of our knowledge, there is no report of tripodal trinuclear s-triazine cored lanthanide salen Schiff base complexes. There is also no report on their applications in biological studies.
Neodymium is one of the lanthanides and has electronic configuration of [Xe] 4f⁴5d⁰ 6s². It has many industrial applications viz: permanent magnets (Emsley, 2011), lasers (Norman et al., 2002) and glass (Bray, 2001). A survey through literature has shown that neodymium complexes with various organic ligands possess interesting properties such as cytotoxic (Manolov et al., 1999; Kostova et al., 2004), antitumour (Kostova et al., 1999; Kostova et al., 2001), anticoagulant (Kostova and Nikolova, 2006), and antimicrobial (Oruma et al., 2014; Taha et al., 2011) activities. Based on these findings, we decided to synthesize, characterize and study the biological activities of Nd(III) salen capped complex with 2,4,6-tris(4-carboxybenzimino)-1,3,5-triazine.

MATERIALS AND METHODS

Materials and Measurements

Chemicals used were of analytical reagent grade and were purchased from Zayo–Sigma. They were used as supplied without further purification. Fischer Jones melting point apparatus was used for determining the melting points of the compounds and were uncorrected. Molar conductance measurements were carried out with WTW-LF 90 conductivity meter by dissolving 10⁻⁴ mol/L solutions of the complex in methanol at room temperature. Electronic spectra were recorded on UV-Vis 1800 SHIMADZU spectrophotometer in dimethyl sulfoxide (DMSO). A Perkin–Elmer (Waltham, Massachusetts, USA) 100 series version 10.03.08 FTIR spectrophotometer was used to run the Infrared spectra of the compounds. The ¹H and ¹³C NMR spectra of the compounds were recorded on a Bruker (Billerica, Massachusetts, USA) DPX 300 spectrometer in DMSO- d₆ at 300.13MHz and 75.47MHz, respectively. Elemental analysis for C, H and N were carried out using LECO – CHN – 932 analyzer.

Synthesis of 2,4,6-tris(4-carboxybenzimino)-1,3,5-triazine(H₃MT)

The method reported by Uysal and Ucan (2009) (Uysal and Ucan, 2009) was adopted. 2,4,6-triamino-1,3,5-triazine (0.63 g, 0.005 mol) was dissolved in benzene (5 mL) stirred for 1 h, then 4-carboxybenzaldehyde (2.25 g, 0.015 mole) added and refluxed for 4 h. A white precipitate was obtained, filtered, and recrystallized from a mixture of methanol and water, dried and stored over CaCl₂. See Scheme 1.

Scheme 1: Synthesis of 2,4,6-tris(4-carboxybenzimino)-1,3,5-triazine (H₃MT).
Synthesis of [Nd(III)(salen)] Capped Complex of 2,4,6-tris(4-carboxybenzimino)-1,3,5-triazine

Nd(III)LC (0.33 g, 0.00037 mol) was suspended in hot absolute ethanol (25 mL) and a solution of H₃MT (0.13 g, 0.00025 mol) in absolute ethanol was added while stirring. The reaction mixture was boiled under reflux for 4 h. The light yellow solid formed was dried over CaCl₂. See Scheme 2.

Synthesis of Precursors

Synthesis of SalenH₂

SalenH₂ was synthesized by modifying the method reported by Sathe et al., (Sathe et al., 2013). To a solution of ethylenediamine (3.35 mL, 0.05 mol) in 50 mL of methanol in a round bottom flask, salicylaldehyde (10.47 mL, 0.1 mol) was added. The yellow crystalline solid produced was filtered and recrystallized from absolute ethanol (50 mL) at 80 °C.

The UV and IR spectra are presented in supplementary materials (Figures S1 and S6). Yield = 11.14 g (83 %); mp of 109–110 °C; UV (λnm) (DMSO) (ε): 316 (1.91 × 10⁴), 404 (0.41 × 10⁴); IR (KBr): 3441 (br) ((O−H) Phenolic), 1608 (s) (C= N), 1287 (m) (C−O), 751 (m) (C−H) cm⁻¹; Anal. calcd for C_{16}H_{16}O_{2}N_{2} (268): C, 71.64; H, 5.97; N, 10.45. Found: C, 71.60; H, 6.00; N, 10.30.

Synthesis of Nd(III) Salen Complex

The method reported by Gembický et al., (Gembický et al., 2000) was modified and adopted for synthesis of salen complexes. To a hot methanolic solution (40 mL) of salenH₂ (1.34 g, 0.005 mol), a hot methanolic solution (50 mL) of neodymium(III) nitrate pentahydrate, Nd(NO₃)₃.5H₂O (2.09 g, 0.005 mol) was added. An orange-colored solution was formed. The mixture was stirred at 50 °C for 30 min., and then triethylamine (0.02 mol, 4 mL) was added. On adding triethylamine, the color changed from orange to milky color.

The resulting solution was stirred at 50 °C for 2 h and after cooling a milk-colored precipitate was formed. The precipitate was washed with methanol and diethyl ether and dried over CaCl₂. Yield = 2.20 g (73.58 %); mp of 280° (a = decomposition temperature) °C; UV (DMSO) λmax nm (ε): 271 (9.39 x10⁴), 318 (7.60 x10⁴); IR (KBr): 3432 (O−H), 1630 (C=N), 1189 (C−O), 1452, 1049,884 (NO₃⁻), 756 (C−H), 579 (Ln−O), 399 (Ln−N); ¹H NMR spectrum could not be taken due to their paramagnetic character; Anal. Calcd for [Nd(H₂L)(NO₃)₃]NO₃ (598.24): C, 32.09; H, 2.67; N, 11.70. Found: C, 32.30; H, 2.80; N, 11.84. The UV and IR spectra are presented in supplementary materials (Figures S2 and S7).

\[
\begin{align*}
\text{SalenH}_2 + \text{Nd(NO}_3)_3 \cdot 5\text{H}_2\text{O} \rightarrow \text{[Nd(H}_2\text{L})(\text{NO}_3)_3\text{]}\text{NO}_3 \cdot 5\text{H}_2\text{O}
\end{align*}
\]

\[M = \text{Nd}, \; X = \text{OH}\]

Scheme 2: Synthesis of [(Nd(OH)₂(salen))₃(MT)]₃H₂O.
Synthesis of Nd(III) Ligand Complex (Nd(III)LC)

The ligand complexes were prepared by modifying the method reported by Kopel et al., (Kopel et al., 1998). A solution of Nd(III) salen complex (0.50 g, 10^{-3} mol) in absolute ethanol (20 mL) was stirred at 50 °C for 15 min. Excess concentrated ammonia solution (1 mL at a time) was added and stirred. The pH of the solution was monitored with the aid of a pH meter until the pH of 12. A greyish yellow precipitate was formed, filtered and dried over CaCl_2. Yield = 0.34 g (48.57 %); mp of 205 °C; UV (DMSO) \( \lambda_{max} \text{nm (} \varepsilon \text{): 263 (13.2 \times 10^3), 318 (5.54 \times 10^3)} \); IR (KBr): 3500 (O-H), 1623 (C=N), 1553 (C=C), 1296 (C-O), 851, 753 (C-H), 597 (Ln-O-Ln), 571 (Ln-O); ^1H NMR spectrum could not be taken due to their paramagnetic character; Anal. Calcd for \([\text{Nd(OH)}_2(\text{salen})_2\text{O}]\) (904.48): C, 42.46; H, 3.54; N, 6.19. Found: C, 42.50; H, 3.62; N, 6.23. The UV and IR spectra are presented in supplementary materials (Figures S3 and S8).

In vitro Antimicrobial Activity

The in vitro antimicrobial activities of H_3MT and its trinuclear Nd(III) salen capped complex were tested against American Type Culture Collection (ATCC) bacteria strains obtained from Rockville, MD, USA, by the Department of Microbiology, University of Nigeria, Nsukka while the fungi strains were isolated under clinical conditions. The typed bacteria culture comprises Gram- positive bacteria: Staphylococcus aureus (ATCC 6538P) and Bacillus cereus (ATCC 14579); Gram- negative bacteria: Escherichia coli (ATCC 6749) and Pseudomonas aeruginosa (ATCC 9027). The fungi strains used were Candida albicans and Aspergillus niger. The bacteria strains were tested for sterility on nutrient agar and then grown in nutrient broth at 37 °C for 24 hours while the fungal strains were tested on Sabourand Dextrose Agar (SDA) and cultured in Sabourand Dextrose Liquid medium at 25 °C for 24 hours. The overnight cultures were subsequently diluted and suspensions were made in normal saline and adjusted to 0.5 McFarland standards (Cheesbrough, 2006).

Antimicrobial Assay

Agar cup diffusion technique (Alli et al., 2011) was employed to determine the antimicrobial activities of H_3MT and its trinuclear Nd(III) salen capped complex. The nutrient agar and SDA plates were inoculated with 0.1 mL broth culture of the test bacteria or fungi. Using a sterile cork borer, wells (5 mm in diameter and 2.5 mm deep) were bored into the inoculated agar. Fresh stock solutions (1000 μg/mL) of the synthesized compounds were prepared in DMSO. The stock solution was further diluted with sterilized distilled water to 12.5, 25, and 50 μg/mL for antimicrobial evaluation. The wells were filled with 100 μL of the test compounds by means of a sterile micropipette. Standard antibiotics namely: ciprofloxacin, tetracycline, gentamycin and fluconazole were used as positive control while sterile DMSO served as negative control. Subsequently, 12.5, 6.25, and 3.125 μg/mL of each positive control were prepared in DMSO. The bacteria plates were incubated at 37 °C for 24 hours while fungal plates were incubated at 25 °C for 24 hours. Inhibition zone diameter (IZD) around each well was measured in millimeter and recorded. The graph of IZD^2 against the log of concentration was plotted for each plate containing a specific compound and a microorganism. The anti-log of the intercept on x-axis is the MIC.

RESULTS AND DISCUSSION

Synthesis of Nd(III) salen capped complex of 2,4,6-tris(4-carboxybenzimino)-1,3,5-triazine involves four steps namely synthesis of: salenH_2, Nd(III) complex, Nd(III)LC, and \([\text{Nd(OH)}_2(\text{salen})_3(\text{MT})]\).3H_2O. Synthesis of H_3MT and its trinuclear Nd(III) salen capped complex was achieved in high yield (86.21 %) and (95.56 %), respectively. These compounds are soluble in DMSO, DMF, ethylacetate, and methanol but insoluble in water. The analytical data of H_3MT and its trinuclear Nd(III) salen capped complex are in good agreement with the proposed molecular formula as shown in Table 1. Molar conductivity measurements in methanol at room temperature indicate that both compounds are neutral (Ali et al., 2013).

Electronic Spectra

The UV/Vis absorption spectra of the H_3MT and \([\text{Nd(OH)}_2(\text{salen})_3(\text{MT})]\).3H_2O (10^{-4} \text{ moldm}^{-3}) were carried out in DMSO at room temperature. The spectral values of the absorption wavelength and the corresponding molar absorbptivities (\(\varepsilon\)) are given in Table 2.
Table 1: Elemental and Physical Data of H3MT and [{Nd(OH)2(salen)}3(MT)].3H2O.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Color</th>
<th>$\Lambda = \nu_{\text{cm}^{-1}}$</th>
<th>Yield g (%)</th>
<th>M.p. (°C)</th>
<th>Molar mass (g/mol)</th>
<th>Elemental analysis % calc. and found</th>
<th>C</th>
<th>H</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>C27H18O6N6 (H3MT)</td>
<td>White</td>
<td>-</td>
<td>(2.25) 86.21</td>
<td>522</td>
<td>346a</td>
<td>62.07</td>
<td>61.95</td>
<td>3.40</td>
<td>3.40</td>
</tr>
<tr>
<td>[{Nd(OH)2(salen)}3(MT)].3H2O</td>
<td>Yellow</td>
<td>14</td>
<td>(0.43) 95.56</td>
<td>1905.72</td>
<td>47.23</td>
<td>47.31</td>
<td>3.62</td>
<td>3.68</td>
<td>8.82</td>
</tr>
</tbody>
</table>

$^a$ = decomposition temperature

Table 2: Electronic Absorption Data of H3MT and [{Nd(OH)2(salen)}3(MT)].3H2O.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>$\epsilon \times 10^4$ (mol$^{-1}$ dm$^3$ cm$^{-1}$)</th>
<th>Band assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>C27H18O6N6 (H3MT)</td>
<td>233</td>
<td>2.88</td>
<td>$\pi-\pi^*$</td>
</tr>
<tr>
<td></td>
<td>291</td>
<td>1.82</td>
<td>$\pi-\pi^*$</td>
</tr>
<tr>
<td>[{Nd(OH)2(salen)}3(MT)].3H2O</td>
<td>329</td>
<td>12.3</td>
<td>$\pi-\pi^*$</td>
</tr>
</tbody>
</table>

The absorption spectra are displayed in supplementary materials Figures S4 and S5, respectively. The absorption band of H3MT showed two bands at 233 and 291 nm assigned to $\pi-\pi^*$ transitions of the benzene rings. In the Nd(III) complex, these bands are red shifted, supporting the coordination of H3MT to the Nd(III) ions.

Infrared Spectra

The relevant stretching frequencies of H3MT and its Nd(III) salen capped complex are shown in Table 3 while the spectra are presented in supplementary materials Figures S9 and S10 respectively. A broad band assignable to $\nu$ O-H was observed in the IR spectrum of Nd(III) complex. The absorption band due to the carboxylic acid C = O, was observed at 1674 cm$^{-1}$ in H3MT (Uysal et al., 2016). This band shifted to higher frequencies of about 24 cm$^{-1}$ in Nd(III) complex suggesting coordination of the ligand complex via the carboxylic acid C = O of H3MT. This was further supported by the vibrations of the COO$^{-}$ group observed at 1405 cm$^{-1}$ in Nd(III) complex and at 1391 cm$^{-1}$ in the ligand (Uysal et al., 2009). Two medium bands assignable to C = N(a) and C = N(b) at 1501 and 1573 cm$^{-1}$ respectively were observed in the IR spectrum of H3MT. However, in Nd(III) complex, three bands were observed: C = N (a) band at 1592 cm$^{-1}$, C = N (b) band at 1635 cm$^{-1}$ and C = N(c) band at 1536 cm$^{-1}$ respectively.

Similar observation has been made in literature (Uysal et al., 2009; 2016; 2012). The C = N(a) and C = N(b) stretching vibration in the complex shifted to higher wavenumber in comparison to the same transition in the ligand. Medium band at 572 cm$^{-1}$ in Nd(III) complex were assigned to $\nu$ (Ln –O) (Taha et al., 2011; Lekha et al., 2014) while band at 435 cm$^{-1}$ were assigned to $\nu$ (Ln – N) (Lekha et al., 2014).
Table 3: IR Band Assignments (cm\(^{-1}\)) for H\(_3\)MT and \([\{\text{Nd(OH)\(_2\)}(\text{salen})\}_3(\text{MT})\}\].3H\(_2\)O.

<table>
<thead>
<tr>
<th>Compound</th>
<th>(\nu) O-H</th>
<th>(\nu) C=O</th>
<th>(\nu) C=N</th>
<th>(\nu) C-C</th>
<th>(\nu) COO(^{-})</th>
<th>(\nu) C-N</th>
<th>(\nu) Ln-O</th>
<th>(\nu) Ln-N</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(_3)MT</td>
<td>-</td>
<td>1674(s)</td>
<td>1501(m(^a))</td>
<td>1422(m)</td>
<td>1391(m)</td>
<td>1168(m)</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>([{\text{Nd(OH)(_2)}(\text{salen})}_3(\text{MT})}].3H(_2)O</td>
<td>3182(br)</td>
<td>1698(m)</td>
<td>1592(s(^a))</td>
<td>1479(m)</td>
<td>1405(s)</td>
<td>1150(m)</td>
<td>572(m)</td>
<td>435(m)</td>
</tr>
</tbody>
</table>

Where \(a = \) from triazine ring; \(b = \) from azomethine linkage; \(c = \) from salen

Table 4: \(^1\)H NMR Data of H\(_3\)MT and \([\{\text{Nd(OH)\(_2\)}(\text{salen})\}_3(\text{MT})\}\].3H\(_2\)O.

<table>
<thead>
<tr>
<th>Compound</th>
<th>OH</th>
<th>CH = N</th>
<th>(H_{\text{aromatic}})</th>
<th>CH(_2) = CH(_2)</th>
<th>(H_{\text{O uncoordinated}})</th>
<th>DMSO</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(_3)MT</td>
<td>10.17(1H,s)</td>
<td>9.77(1H,s)</td>
<td>7.99 - 6.25(4H,m)</td>
<td>-</td>
<td>-</td>
<td>2.50</td>
</tr>
<tr>
<td>([{\text{Nd(OH)(_2)}(\text{salen})}_3(\text{MT})}].3H(_2)O</td>
<td>13.57(1H,s)</td>
<td>8.61(1H,s)</td>
<td>7.40(4H,d), 7.27(2H,s), 6.83(2H,s)</td>
<td>5.96(4H,s)</td>
<td>3.40(2H,s)</td>
<td>2.50</td>
</tr>
</tbody>
</table>

Table 5: \(^{13}\)C NMR Data of H\(_3\)MT and \([\{\text{Nd(OH)\(_2\)}(\text{salen})\}_3(\text{MT})\}\].3H\(_2\)O.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Carboxylic carbon</th>
<th>Azomethine carbon</th>
<th>Carbons on triazine ring</th>
<th>Aromatic carbons</th>
<th>DMSO peak</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(_3)MT</td>
<td>193.47</td>
<td>167.47, 165.75</td>
<td>139.07, 136.98</td>
<td>130.32, 129.92</td>
<td>39.89</td>
</tr>
<tr>
<td>([{\text{Nd(OH)(_2)}(\text{salen})}_3(\text{MT})}].3H(_2)O</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>39.88</td>
</tr>
</tbody>
</table>

The \(^1\)H and \(^{13}\)C NMR spectra of H\(_3\)MT and its Nd(III) salen capped complex are presented in Tables 4 and 5 while the spectra are presented in supplementary materials Figures S11 – S14 respectively. The \(^1\)H NMR spectrum of \([\{\text{Nd(OH)\(_2\)}(\text{salen})\}_3(\text{MT})\}\].3H\(_2\)O is displayed in Figure 1.

The \(^1\)H NMR spectrum of H\(_3\)MT revealed a singlet peak at 10.17 ppm due to carboxylic proton. In \([\{\text{Nd(OH)\(_2\)}(\text{salen})\}_3(\text{MT})\]\].3H\(_2\)O, a singlet peak was observed at 13.57 ppm, and was assigned to OH from Nd(III)LC. The signal due to azomethine protons was observed between 9.77 – 8.29 ppm in the compounds. The signals in the range 6.25 – 7.99 ppm in the compounds were assigned to aromatic protons. The signal due to ethylene protons appeared only in the complex at 5.96 ppm. The spectra revealed the presence of uncoordinated water in the complex.

The \(^{13}\)C NMR of H\(_3\)MT gave signal at 193.47 ppm attributed to carboxylic carbon (Silverstein et al., 2005). The signal due to azomethine carbon was observed at 165.75 and 167.47 ppm in H\(_3\)MT while the signal at 139.07 and 136.98 ppm in H\(_3\)MT has been assigned to carbons on triazine ring. Carbons on benzene ring are present at 130.32 and 129.92 ppm in H\(_3\)MT. The \(^{13}\)C NMR spectrum of \([\{\text{Nd(OH)\(_2\)}(\text{salen})\}_3(\text{MT})\}\].3H\(_2\)O showed only solvent peak probably due to paramagnetism of the Nd(III) ions (Karatas and Ucan, 2014, \(\ddot{I}\)şci and Uysal, 2018).
The results of the in vitro antimicrobial screening carried out on the compounds are recorded in Table 6. Ciprofloxacin, tetracycline, gentamicin and fluconazole were used as positive control while sterile DMSO served as negative control. These drugs have been chosen because they have same mechanism of action, which is by inhibiting nucleic acid synthesis (Oruma et al., 2018).

The results obtained (Table 6) show that the activity of H3MT is higher than that of the trinuclear Nd(III) complex. H3MT exhibits higher activity against fungi (Candida albicans and Aspergillus niger) relative to the bacteria strains used. Hence, it could be inferred that the activity
of the Nd(III) trinuclear complex was not enhanced after anion coordination.

The minimum inhibitory concentration (MIC) of the compounds and controls against *Bacillus cereus*, *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Escherichia coli*, *Candida albicans*, and *Aspergillus niger* are displayed in Table 7. From Table 7, the MIC of [{Nd(OH)₂(salen)}₃(MT)].₃H₂O is 50 μg/mL. This means that below 50 μg/mL, the complex will show no inhibition. The MIC of H₃MT against *Staphylococcus aureus* was 5.57 mg/ml while that of gentamycin was 2.70 mg/ml. The MIC of H₃MT against *Candida albicans* is comparable to that of gentamycin. H₃MT was found to be the most active against *Candida albicans* and *Aspergillus niger* (MIC = 2.60 and 2.30 mg/ml, respectively). However, the standard antifungal drug, Fluconazole was more active against *Candida albicans* and *Aspergillus niger* (MIC = 0.64 and 0.74 mg/ml respectively) relative to H₃MT.

**CONCLUSION**

A new trinuclear Nd(III) salen capped complex derived from 2,4,6-tris(4-carboxybenzimino)-1,3,5-triazine was synthesized and characterized. Based on analytical and spectral data, the ligand was found to be hexadentate and coordinate to Nd(III) ions through the oxygen atoms of the deprotonated carboxylic group. The trinuclear Nd(III) salen capped complex was characterized as being bridged by carboxylate anions to the Nd(III) salen centers and displays a coordination number of eight by involving two hydroxyl groups in the coordination sphere. *In vitro* antimicrobial test indicates that the trinuclear Nd(III) salen capped complex inhibits the growth of *Bacillus cereus*, *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Escherichia coli*, *Candida albicans*, and *Aspergillus niger* at concentrations of 50 μg/mL.

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**Table 7: Minimum Inhibitory Concentration (MIC) of the Compounds and Controls against Test Bacteria and Fungi.**

<table>
<thead>
<tr>
<th>Compound</th>
<th>B.c (ATCC 14579)</th>
<th>S.a (ATCC 6538P)</th>
<th>P.a (ATCC 9027)</th>
<th>E.c (ATCC 6749)</th>
<th>C.a</th>
<th>A.n</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₃MT</td>
<td>50</td>
<td>5.57</td>
<td>6.27</td>
<td>7.3</td>
<td>2.6</td>
<td>2.3</td>
</tr>
<tr>
<td>[{Nd(OH)₂(salen)}₃(MT)].₃H₂O</td>
<td>50</td>
<td>50</td>
<td>50</td>
<td>50</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>Controls</td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>T</td>
<td>1.90</td>
<td>1.80</td>
<td>0.63</td>
<td>2.15</td>
<td>2.10</td>
<td>0.58</td>
</tr>
<tr>
<td>F</td>
<td>6.25</td>
<td>6.25</td>
<td>6.25</td>
<td>2.80</td>
<td>0.64</td>
<td>0.74</td>
</tr>
<tr>
<td>CP</td>
<td>1.50</td>
<td>0.70</td>
<td>0.92</td>
<td>0.65</td>
<td>2.00</td>
<td>6.25</td>
</tr>
<tr>
<td>G</td>
<td>1.40</td>
<td>2.70</td>
<td>0.71</td>
<td>2.60</td>
<td>2.50</td>
<td>0.64</td>
</tr>
</tbody>
</table>

Legend: T = Tetracycline, F = Fluconazole, CP = Ciprofloxacin, G = Gentamycin.
SUPPLEMENTARY MATERIALS

Figure S1: Electronic Absorption Spectrum of SalenH₂.

Figure S2: Electronic Absorption Spectrum of Nd(III)Salen Complex.
**Figure S3:** Electronic Absorption Spectrum of Nd(III) Ligand Complex.

**Figure S4:** Electronic Absorption Spectrum of H₃MT.
Figure S5: Electronic Absorption Spectrum of \([\text{Nd(OH)}_2(\text{salen})_3(\text{MT})]\cdot3\text{H}_2\text{O}\).

Figure S6: Infrared Spectrum of SalenH₂.

Figure S7: Infrared Spectrum of Nd(III)Salen Complex.
Figure S8: Infrared Spectrum of Nd(III) Ligand Complex.

Figure S9: Infrared Spectrum of H₃MT.
Figure S10: Infrared Spectrum of [(Nd(OH)₂(salen))₃(MT)].3H₂O.

Figure S11: 'H NMR Spectrum of H₃MT.
Figure S12: $^1$H NMR Spectrum of [Nd(OH)$_2$(salen)]$_3$(MT)].3H$_2$O.

Figure S13: $^{13}$C NMR Spectrum of H$_3$MT.
REFERENCES


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