Electronic Supporting Information

Supporting Information for ‘Plasma Deposited Metal Schiff-base Compounds as Antimicrobials’

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Structure solution refinement

Experimental details relating to the single-crystal X-ray crystallographic studies are summarized in table 2. For both structures, data were collected on a Nonius Kappa CCD diffractometer at 150(2) K using Mo-K\textsubscript{\textalpha} radiation (\(\lambda = 0.71073\) Å). Structure solution and refinements were performed using SHELX86\textsuperscript{i} and SHELX97\textsuperscript{ii} software, respectively. Corrections for absorption were made in all cases. For all complexes, hydrogen atoms were included at calculated positions.
Crystal structure data for ZSB and CSB compounds

Table S1: Crystallographic data for the complexes ZSB and CSB.

<table>
<thead>
<tr>
<th>Compound</th>
<th>ZSB</th>
<th>CSB</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>$C_{20}H_{20}ZnN_2O_2$</td>
<td>$C_{20}H_{20}CuN_2O_2$</td>
</tr>
<tr>
<td>Formula weight</td>
<td>385.75</td>
<td>383.92</td>
</tr>
<tr>
<td>T/K</td>
<td>150(2)</td>
<td>150(2)</td>
</tr>
<tr>
<td>Crystal system</td>
<td>Triclinic</td>
<td>Monoclinic</td>
</tr>
<tr>
<td>Space group</td>
<td>$P\bar{1}$</td>
<td>$P2_1/c$</td>
</tr>
<tr>
<td>$a$ / Å</td>
<td>9.8230(5)</td>
<td>10.7130(2)</td>
</tr>
<tr>
<td>$b$ / Å</td>
<td>10.3560(6)</td>
<td>7.3560(10)</td>
</tr>
<tr>
<td>$c$ / Å</td>
<td>10.7400(6)</td>
<td>22.3240(4)</td>
</tr>
<tr>
<td>$\alpha$ / °</td>
<td>63.590(3)</td>
<td></td>
</tr>
<tr>
<td>$\beta$ / °</td>
<td>76.146(3)</td>
<td>102.8980(10)</td>
</tr>
<tr>
<td>$\gamma$ / °</td>
<td>70.354(2)</td>
<td></td>
</tr>
<tr>
<td>$U$ / Å³</td>
<td>916.31(9)</td>
<td>1714.85(5)</td>
</tr>
<tr>
<td>$Z$</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>$D_c$ / g cm⁻³</td>
<td>1.398</td>
<td>1.487</td>
</tr>
<tr>
<td>$\mu$ / mm⁻¹</td>
<td>1.355</td>
<td>1.289</td>
</tr>
<tr>
<td>$F(000)$</td>
<td>400</td>
<td>796</td>
</tr>
<tr>
<td>Crystal size / mm</td>
<td>0.30, 0.10, 0.10</td>
<td>0.2, 0.17, 0.13</td>
</tr>
<tr>
<td>Theta range / °</td>
<td>3.95 to 27.61</td>
<td>8.54 to 28.28</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>11966</td>
<td>24844</td>
</tr>
<tr>
<td>Reflections ([I&gt;2\sigma(I)])</td>
<td>4188 ([R(\text{int}) = 0.0705])</td>
<td>4117 ([R(\text{int}) = 0.1017])</td>
</tr>
<tr>
<td>Data / restraints / parameters</td>
<td>4188/0/226</td>
<td>4117/0/227</td>
</tr>
<tr>
<td>Goodness of fit</td>
<td>1.105</td>
<td>1.039</td>
</tr>
<tr>
<td>Final $R1$ ($wR_2$) ([I&gt;2\sigma(I)])</td>
<td>0.0527 (0.1258)</td>
<td>0.0339 (0.0856)</td>
</tr>
<tr>
<td>Final $R1$ ($wR_2$) (all data)</td>
<td>0.0741 (0.1400)</td>
<td>0.0439 (0.0910)</td>
</tr>
<tr>
<td>Largest diff. peak and hole, eÅ⁻³</td>
<td>1.145 and -0.661</td>
<td>0.336 and -0.399</td>
</tr>
</tbody>
</table>
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Selected Bond lengths (Å) and angles (°)

<table>
<thead>
<tr>
<th></th>
<th>ZSB</th>
<th>CSB</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zn(1)-O(1)</td>
<td>1.988(2)</td>
<td>Cu(1)-O(1)</td>
</tr>
<tr>
<td>Zn(1)-O(2)</td>
<td>2.085(2)</td>
<td>Cu(1)-O(2)</td>
</tr>
<tr>
<td>Zn(1)-N(1)</td>
<td>2.051(3)</td>
<td>Cu(1)-N(1)</td>
</tr>
<tr>
<td>Zn(1)-N(2)</td>
<td>2.070(3)</td>
<td>Cu(1)-N(2)</td>
</tr>
<tr>
<td>Zn(1)-O(2) #</td>
<td>2.048(2)</td>
<td></td>
</tr>
<tr>
<td>O(1)-Zn(1)-O(2)</td>
<td>171.91(9)</td>
<td>O(1)-Cu(1)-O(2)</td>
</tr>
<tr>
<td>N(1)-Zn(1)-N(2)</td>
<td>110.49(10)</td>
<td>N(1)-Cu(1)-N(2)</td>
</tr>
<tr>
<td>N(1)-Zn(1)-O(2) #</td>
<td>122.65(11)</td>
<td>O(1)-Cu(1)-N(1)</td>
</tr>
<tr>
<td>N(2)-Zn(1)-O(2) #</td>
<td>125.62(10)</td>
<td>O(2)-Cu(2)-N(2)</td>
</tr>
<tr>
<td>O(1)-Zn(1)-N(1)</td>
<td>91.27(10)</td>
<td>O(1)-Cu(2)-N(2)</td>
</tr>
<tr>
<td>C(7)-N(1)</td>
<td>1.290(4)</td>
<td>C(7)-N(1)</td>
</tr>
<tr>
<td>C(17)-N(2)</td>
<td>1.287(4)</td>
<td>C(27)-N(2)</td>
</tr>
<tr>
<td>Zn(1)-O(2)-Zn(1) #</td>
<td>103.79(9)</td>
<td></td>
</tr>
</tbody>
</table>

|      | # 1-x+2,-y,-z |

Table S2: Selected Bond Distances (Å) and Bond Angles (deg) for the Complexes ZSB and CSB. a
Symmetry transformations used to generate equivalent atoms: # 1 -x+2,-y,-z
**Figure S1**: XPS survey scan of pp-ZSB 1/40 30 min deposition
MIC data for ZSB and CSB compounds

**Staphylococcus aureus MSSA**

**A)** ZSB, Zn acetate & SB ligand

**B)** CSB, Cu acetate & SB ligand

**Pseudomonas aeruginosa PA01**

**C)** ZSB, Zn acetate & SB ligand

**D)** CSB, Cu acetate & SB ligand

**Figure S2:** Bacterial density – concentration plots used for determination of minimum inhibition concentration of compounds.
Figures 3. FTIR of ZSB and CSB monomers and plasma deposited 1/40 films.

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1 Sheldrick, G. M. SHELX-86, Computer Program for Crystal Structure Determination; University of Göttingen: Germany, 1986.