

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 α radiation ($\lambda = 0.71073$ Å). Structure solution and refinements were performed using SHELX86ⁱ and SHELX97ⁱⁱ software, respectively. Corrections for absorption were made in all cases. For all complexes, hydrogen atoms were included at calculated positions.

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Crystal structure data for ZSB and CSB compounds

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

Compound	ZSB	CSB
Formula	C ₂₀ H ₂₀ ZnN ₂ O ₂	C ₂₀ H ₂₀ CuN ₂ O ₂
Formula weight	385.75	383.92
T/K	150(2)	150(2)
Crystal system	Triclinic	Monoclinic
Space group	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> / Å	9.8230(5)	10.7130(2)
<i>b</i> / Å	10.3560(6)	7.35600(10)
<i>c</i> / Å	10.7400(6)	22.3240(4)
α / °	63.590(3)	
β / °	76.146(3)	102.8980(10)
γ / °	70.354(2)	
<i>U</i> / Å ³	916.31(9)	1714.85(5)
<i>Z</i>	2	4
<i>D</i> _c / g cm ⁻³	1.398	1.487
μ / mm ⁻¹	1.355	1.289
<i>F</i> (000)	400	796
Crystal size / mm	0.30, 0.10, 0.10	0.2, 0.17, 0.13
Theta range / °	3.95 to 27.61	8.54 to 28.28
Reflections collected	11966	24844
Reflections [<i>I</i> > 2 σ (<i>I</i>)]	4188 [R(int) = 0.0705]	4117 [R(int) = 0.1017]
Data / restraints / parameters	4188/0/226	4117/0/227
Goodness of fit	1.105	1.039
Final <i>R</i> 1 (<i>wR</i> ₂) [<i>I</i> > 2 σ (<i>I</i>)]	0.0527 (0.1258)	0.0339 (0.0856)
Final <i>R</i> 1 (<i>wR</i> ₂) (all data)	0.0741 (0.1400)	0.0439 (0.0910)
Largest diff. peak and hole, eÅ ⁻³	1.145 and -0.661	0.336 and -0.399

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Selected Bond lengths (Å) and angles (°)

ZSB^a			
Zn(1)-O(1)	1.988(2)	O(1)-Zn(1)-O(2)	171.91(9)
Zn(1)-O(2)	2.085(2)	N(1)-Zn(1)-N(2)	110.49(10)
Zn(1)-N(1)	2.051(3)	N(1)-Zn(1)-O(2) #	122.65(11)
Zn(1)-N(2)	2.070(3)	N(2)-Zn(1)-O(2) #	125.62(10)
Zn(1)-O(2) #	2.048(2)		
		O(1)-Zn(1)-N(1)	91.27(10)
C(7)-N(1)	1.290(4)	O(2)-Zn(1)-N(2)	86.05(10)
C(17)-N(2)	1.287(4)		
Zn(1)-O(2)-Zn(1) #	103.79(9)		
CSB			
Cu(1)-O(1)	1.8980(13)	O(1)-Cu(1)-O(2)	176.43(6)
Cu(1)-O(2)	1.8899(13)	N(1)-Cu(1)-N(2)	178.78(6)
Cu(1)-N(1)	2.0126(14)	O(1)-Cu(1)-N(1)	91.19(6)
Cu(1)-N(2)	2.0007(14)	O(2)-Cu(2)-N(2)	92.57(6)
		O(1)-Cu(2)-N(2)	88.25(6)
C(7)-N(1)	1.291(2)	O(2)-Cu(1)-N(1)	88.05(5)
C(27)-N(2)	1.290(2)		

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

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Survey/50

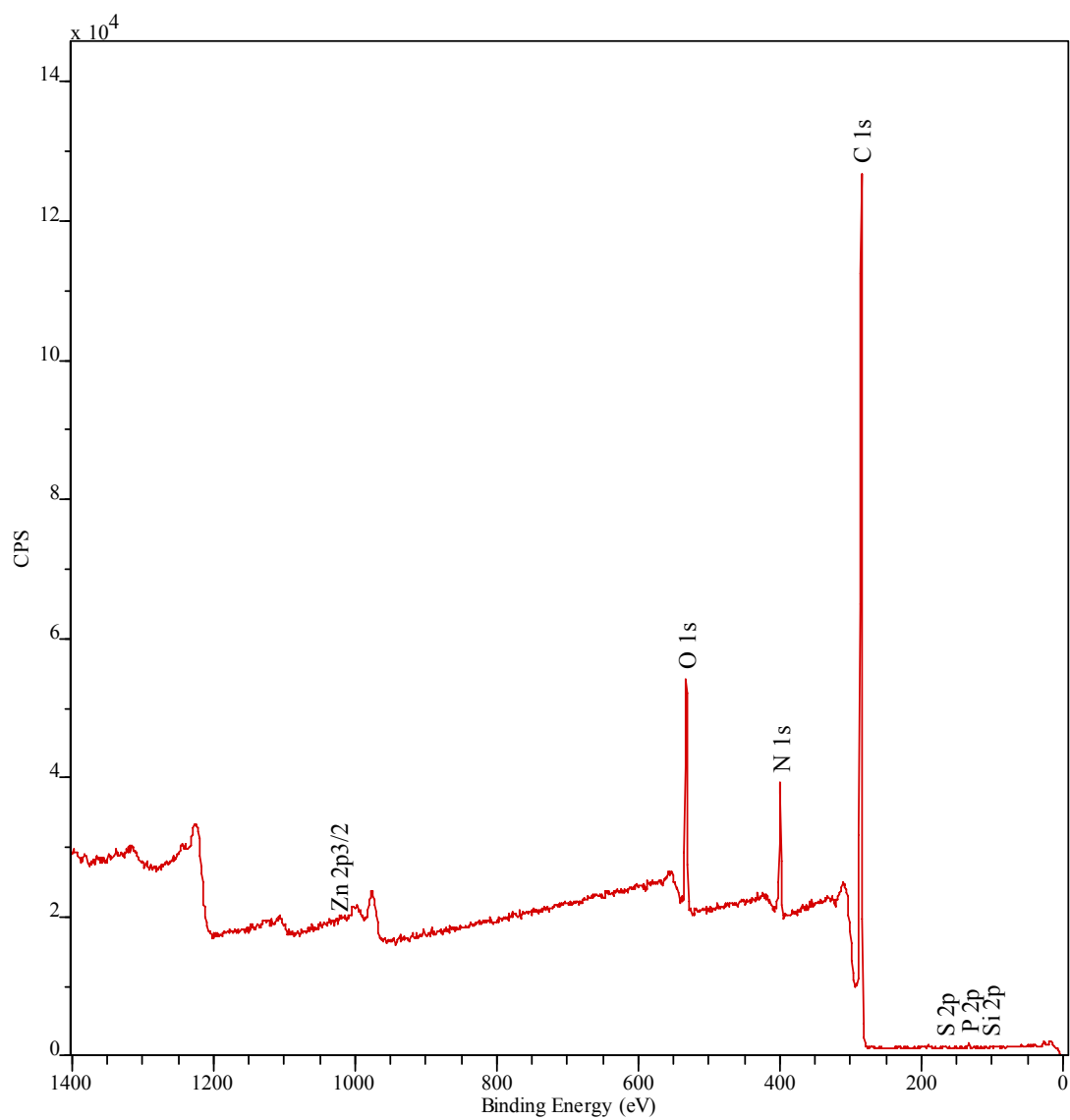


Figure S1: XPS survey scan of pp-ZSB 1/40 30 min deposition

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MIC data for **ZSB** and **CSB** compounds

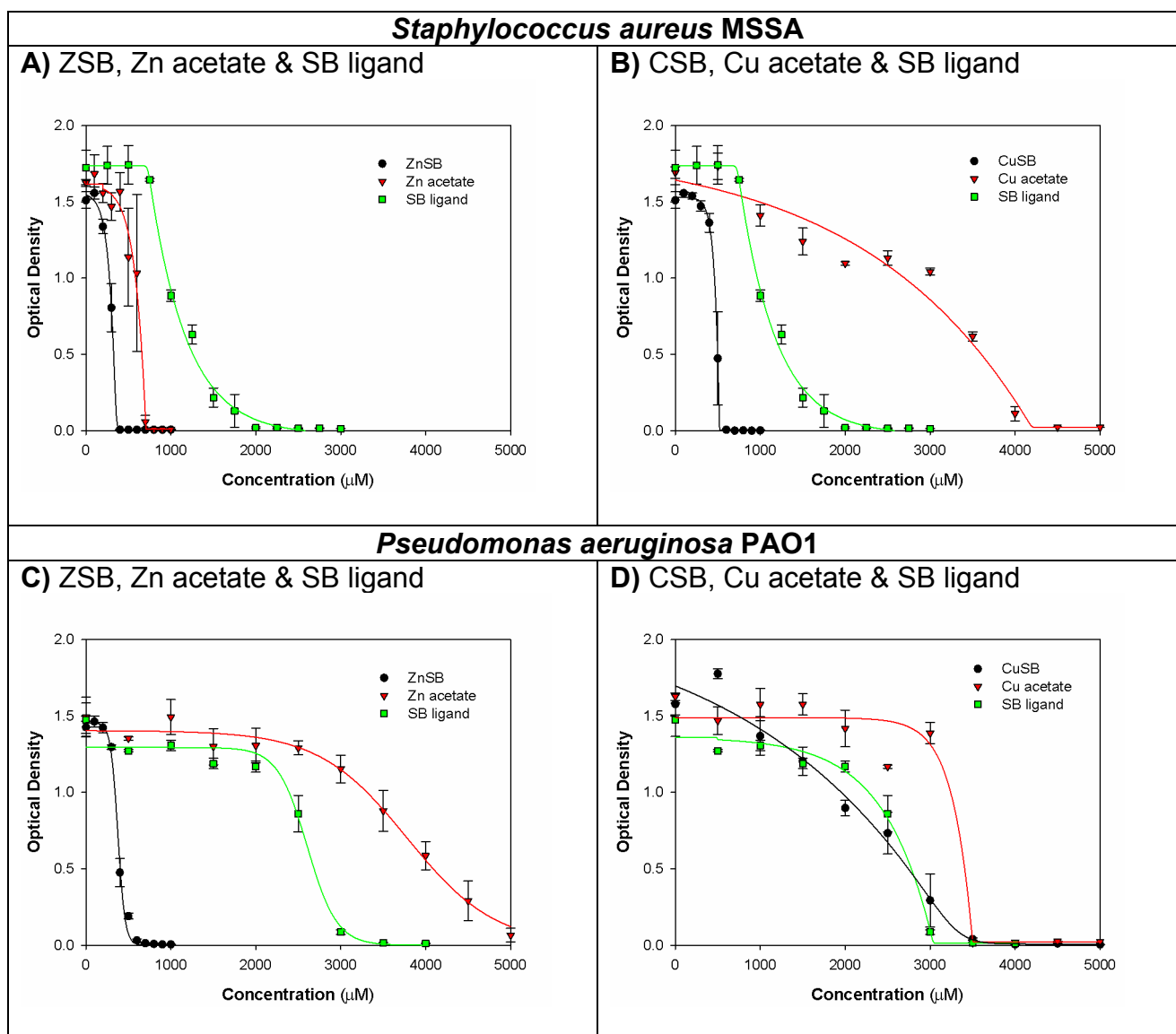
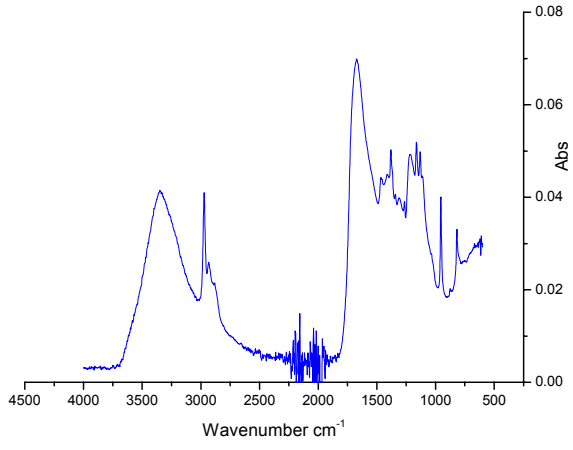
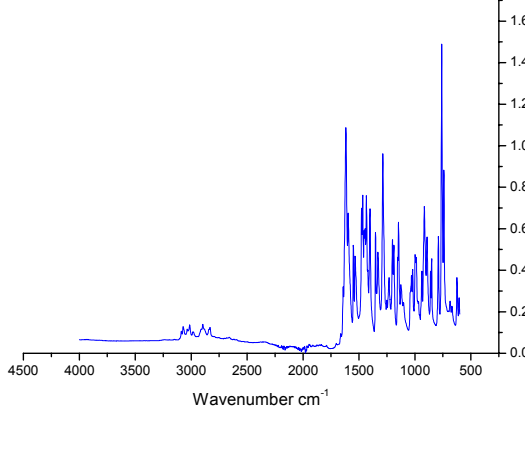
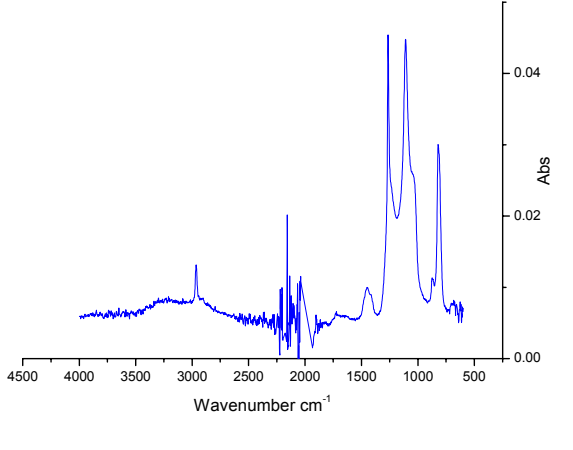
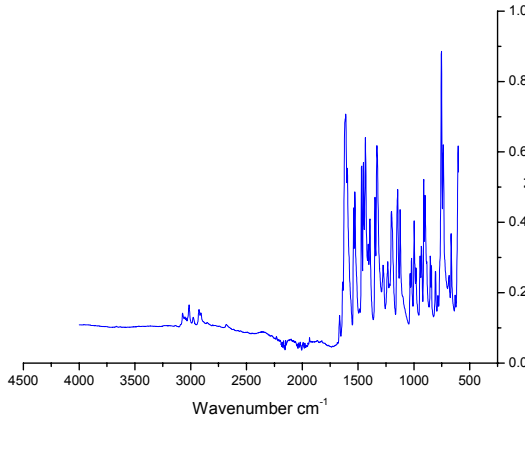


Figure S2: Bacterial density – concentration plots used for determination of minimum inhibition concentration of compounds.

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FTIR of monomers and plasma films

	
ZSB film 1/40	ZSB monomer
	
CSB film 1/40	CSB monomer
Figures3. FTIR of ZSB and CSB monomers and plasma deposited 1/40 films.	

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

ⁱⁱ Sheldrick, G. M. SHELX-97, Computer Program for Crystal Structure Refinement; University of Göttingen: Germany, 1997.