

Supporting Information

Incorporation of a “Two-Tone” Luminescent Silver Complex into Biocompatible Agar Hydrogel composite for Eradication of *ESKAPE* Pathogens in a Skin and Soft Tissue Infection Model

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Table S1 Crystal data and structure refinement parameters for **1** and **2.4H₂O**

	1	2. 4H₂O
Formula	C ₄₈ H ₄₈ Ag ₂ N ₁₀ O ₁₀ S ₂	C ₅₀ H ₅₆ Ag ₂ N ₈ O ₁₄ S ₄ F ₆
$D_{calc.}/\text{g cm}^{-3}$	1.675	1.536
μ/mm^{-1}	0.98	0.84
Formula Weight	1204.82	1450.94
Color	Yellow	Colorless
Shape	Block	Block
T/K	298(2)	298(2)
Crystal System	Triclinic	Monoclinic
Space Group	P-1	P2 ₁ /c
$a/\text{\AA}$	8.9171(6)	16.2215(11)
$b/\text{\AA}$	9.6937(7)	9.3087(6)
$c/\text{\AA}$	14.7140(11)	20.8579(14)
$\alpha/^\circ$	88.179(2)	90
$\beta/^\circ$	86.588(2)	97.828(2)
$\gamma/^\circ$	70.239(2)	90
$V/\text{\AA}^3$	1194.76(15)	3120.2(4)
Z	2	2
Wavelength/ $\text{\AA}$	0.71073	0.71073
Radiation type	Mo-K α	Mo-K α
$2\theta_{min}/^\circ$	6.20	6.00
$2\theta_{max}/^\circ$	56.60	50.20
Measured Refl.	16927	40812
Independent Refl.	5884	5520
Reflections Used	4984	3181
R_{int}	0.020	0.131
Parameters	327	381
^a GooF	1.060	1.070
^c wR_2	0.087	0.196
^b R_I	0.034	0.076

^aGOF = $[\sum[\sum(F_o^2 - F_c^2)^2]/(N_o - N_v)]^{1/2}$ (N_o = number of observations, N_v = number of variables).

^b $R_I = \sum ||F_o| - |F_c|| / \sum |F_o|$. ^c $wR_2 = [(\sum \sum(F_o^2 - F_c^2)^2 / \sum |F_o|^2)]^{1/2}$

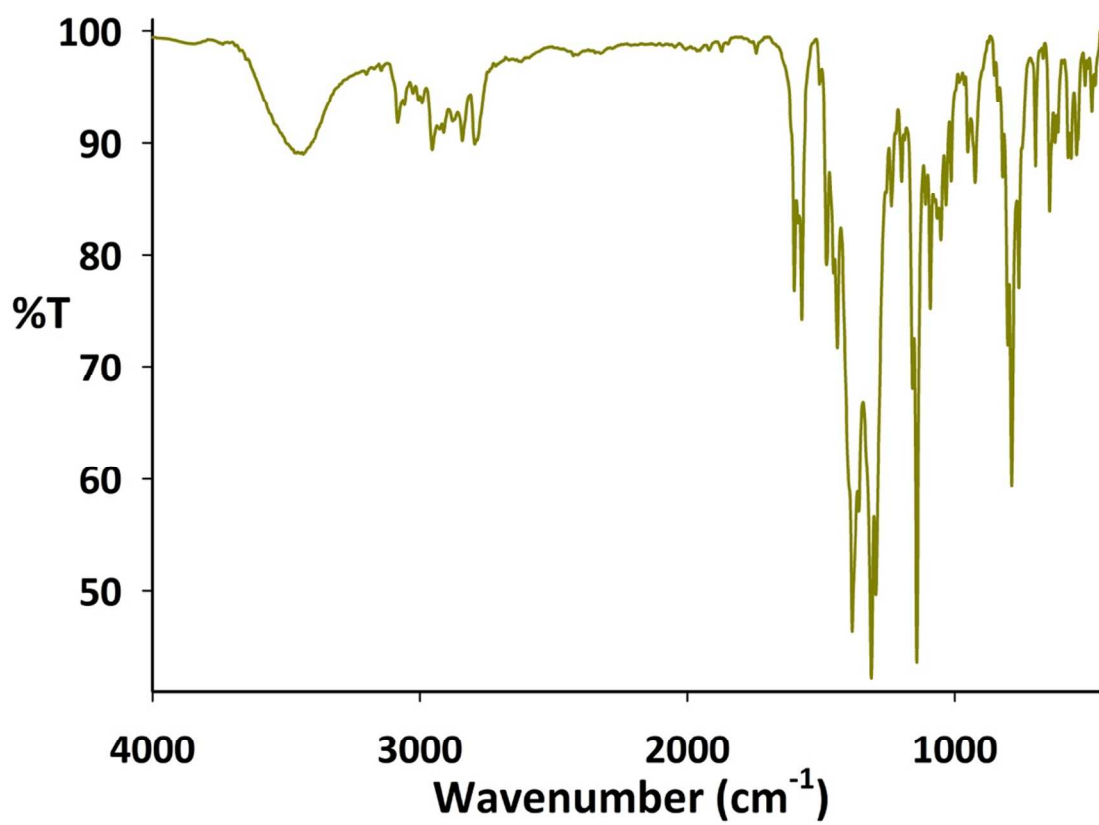


Figure S1 Infrared spectrum (KBr) of $[\text{Ag}_2(\text{DSX})_2(\text{NO}_3)_2]$ (**1**)

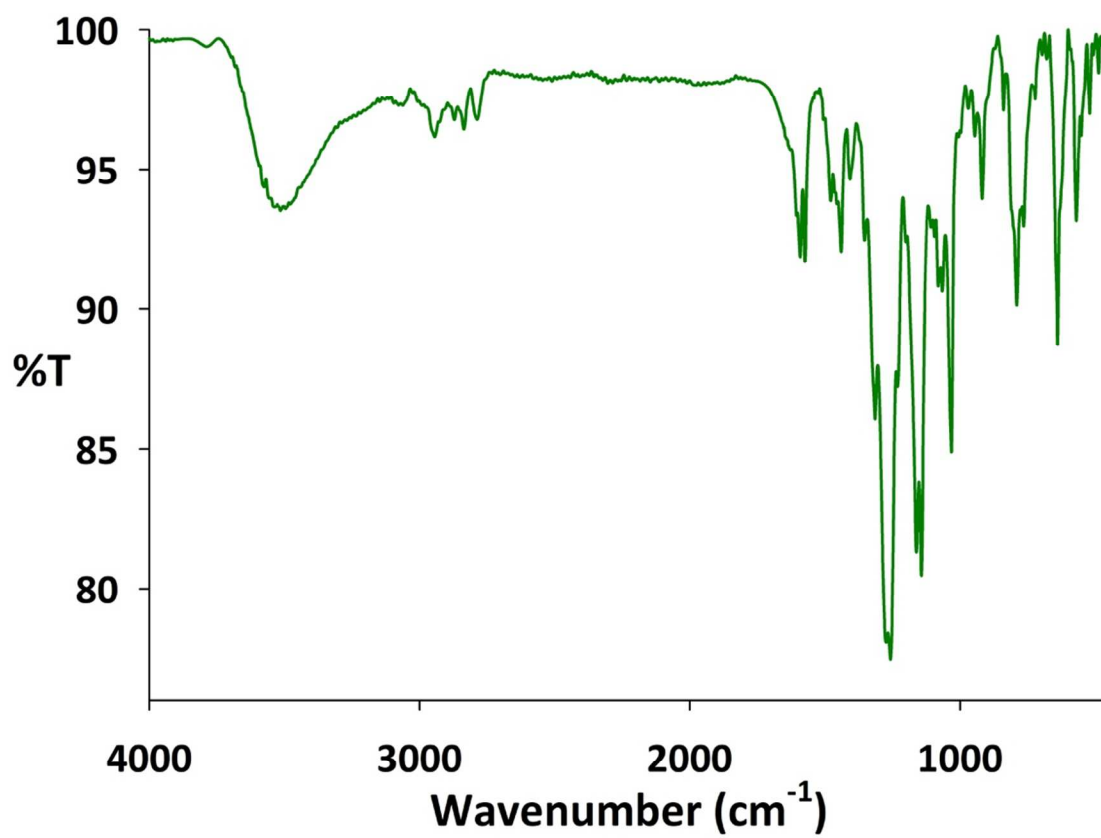


Figure S2 Infrared spectrum (KBr) of $\text{Ag}_2(\text{DSX})_2(\text{CF}_3\text{SO}_3)_2$ (**2**)

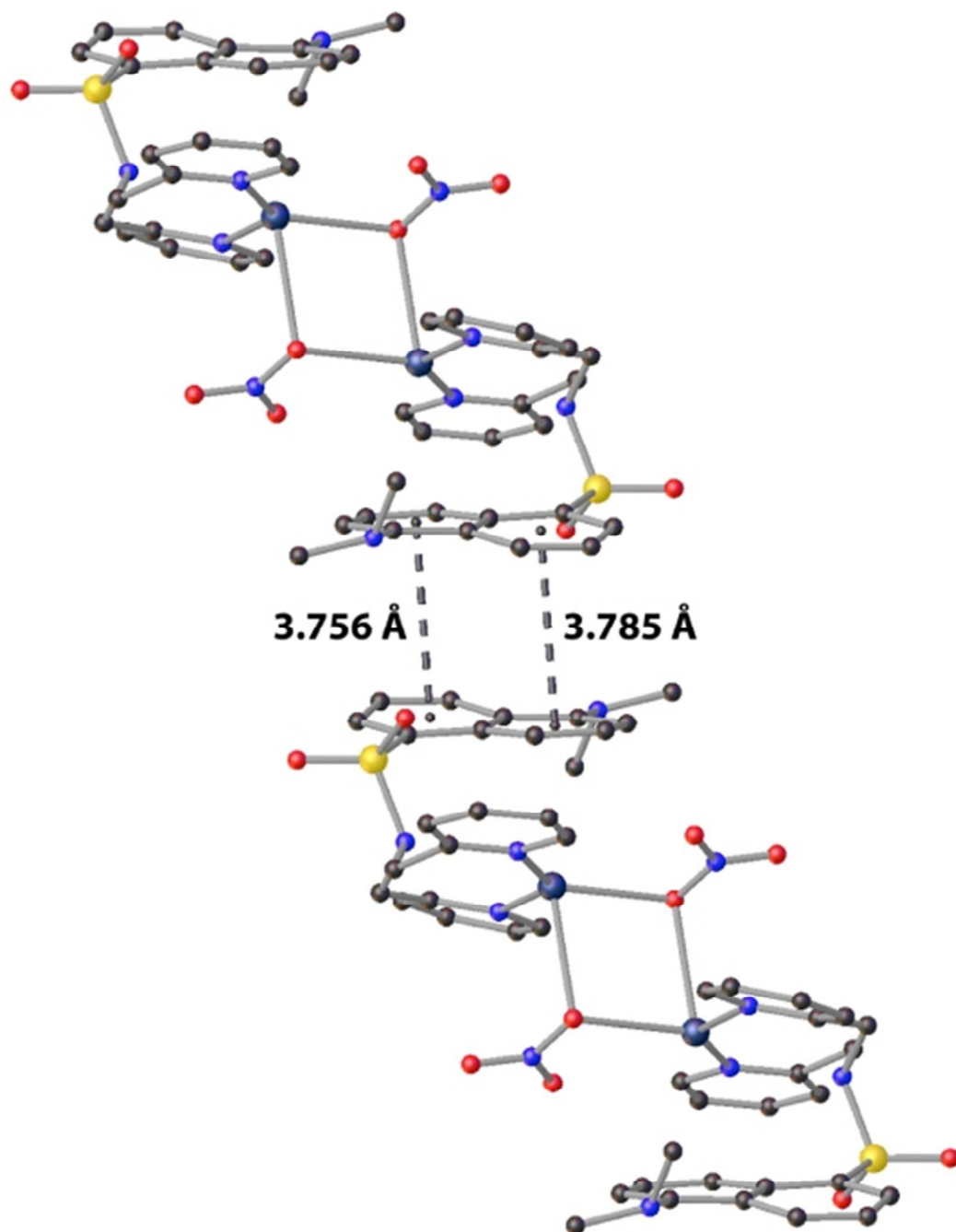


Figure S3 Intermolecular π - π stacking interactions in **1**

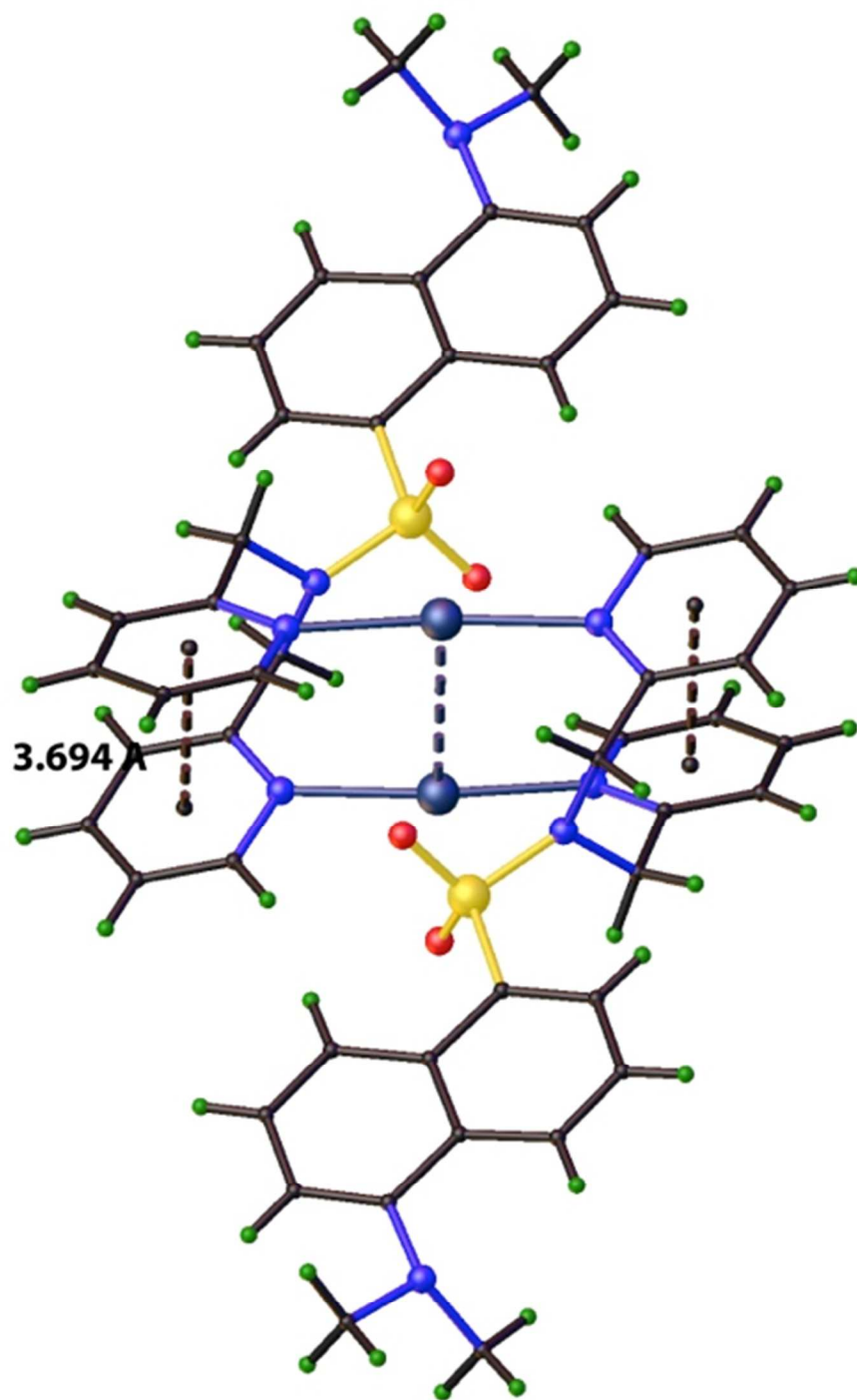


Figure S4 Intramolecular π - π stacking interactions in **2**

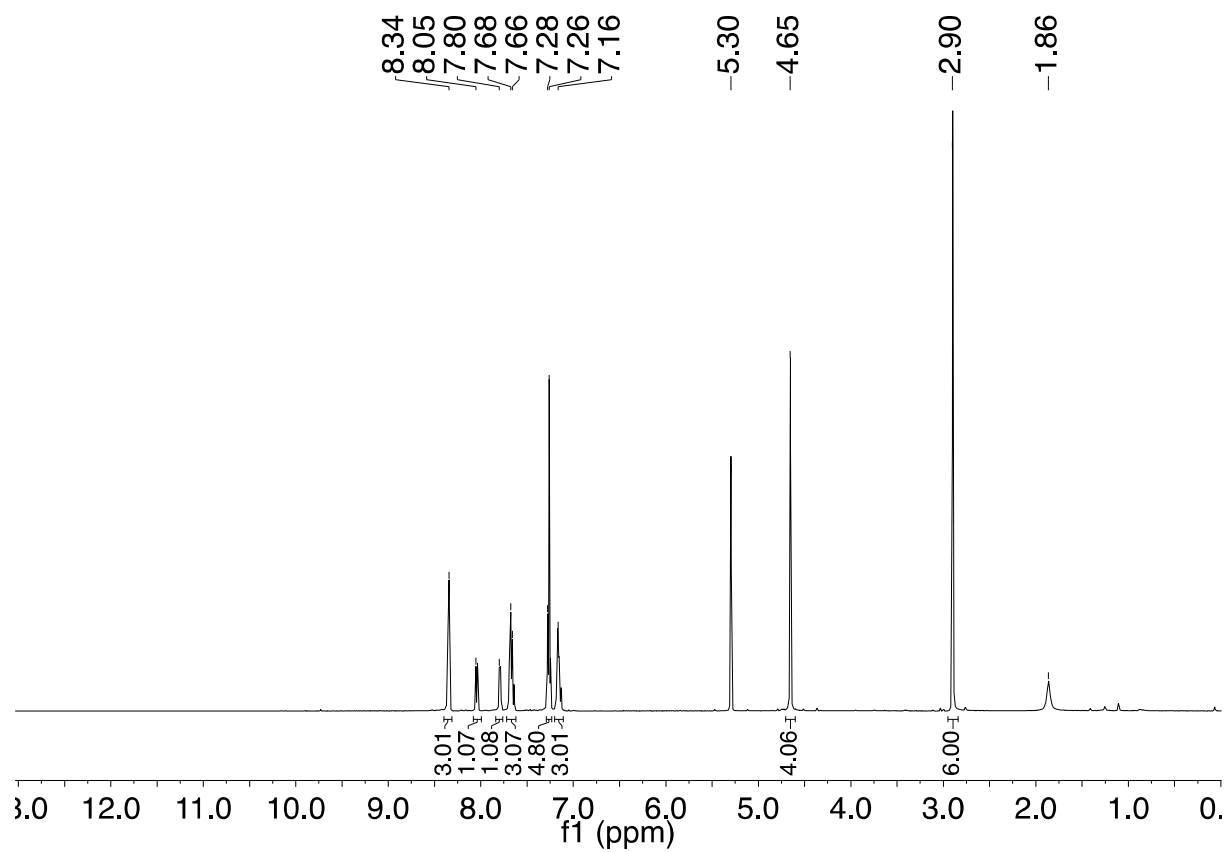


Figure S5 ¹H-NMR (CDCl₃) spectrum of [Ag₂(DSX)₂(NO₃)₂] (**1**)

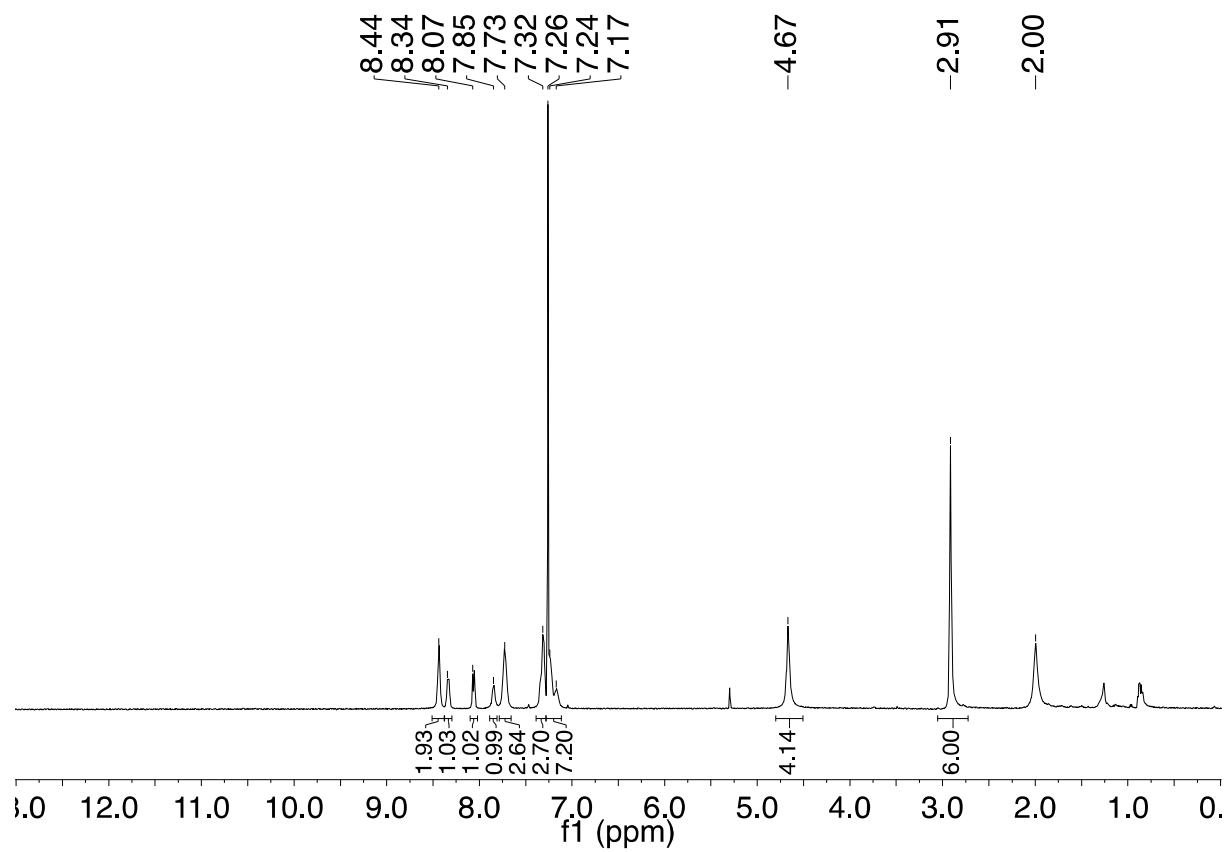


Figure S6 ^1H -NMR (CDCl_3) spectrum of $\text{Ag}_2(\text{DSX})_2(\text{CF}_3\text{SO}_3)_2$ (**2**)

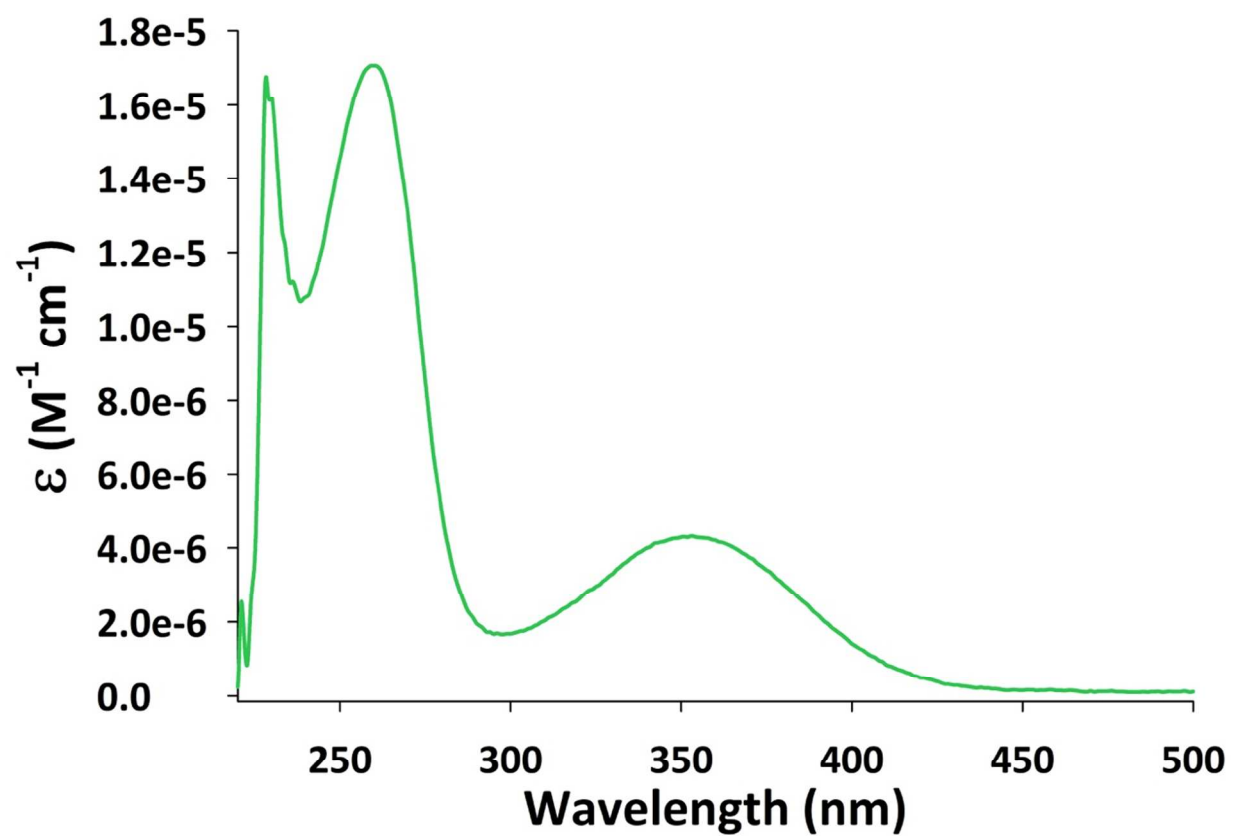


Figure S7 Electronic absorption spectrum of $[Ag_2(DSX)_2(NO_3)_2]$ (**1**) in CH_2Cl_2

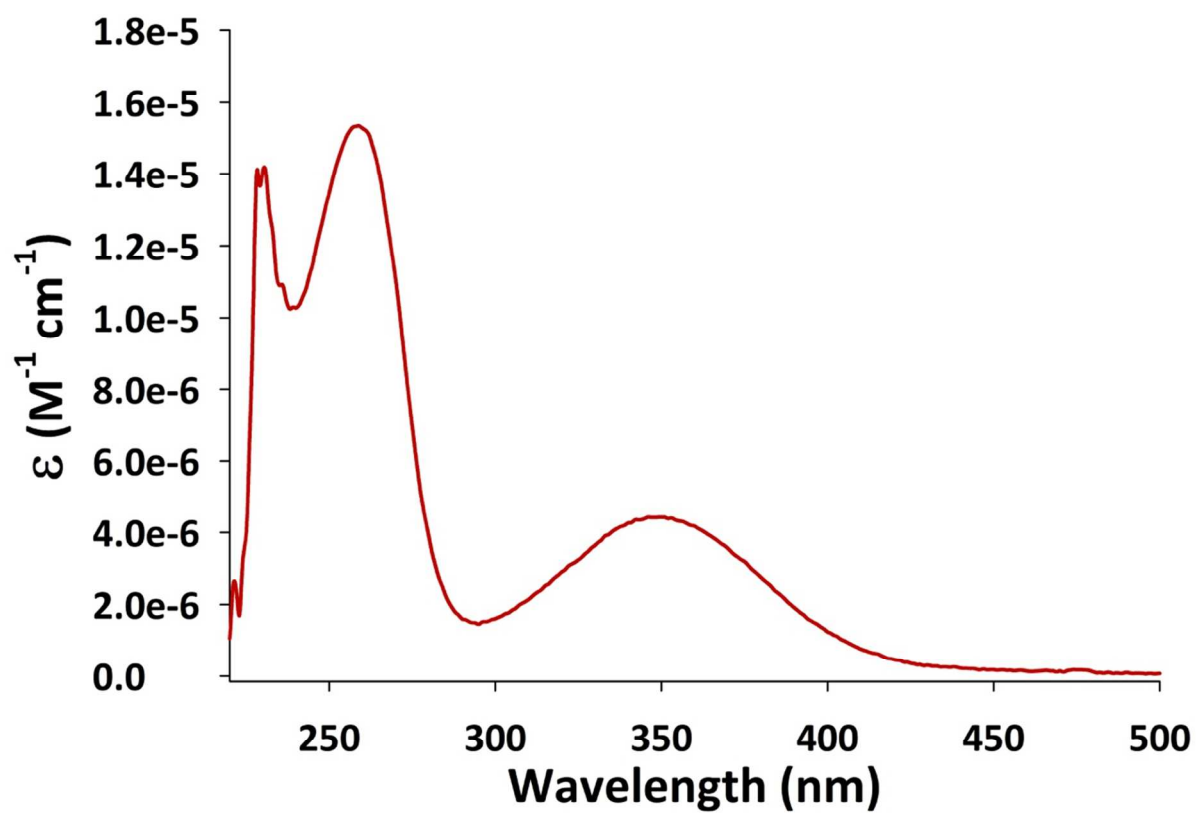


Figure S8 Electronic absorption spectrum of $Ag_2(DSX)_2(CF_3SO_3)_2$ (**2**) in CH_2Cl_2

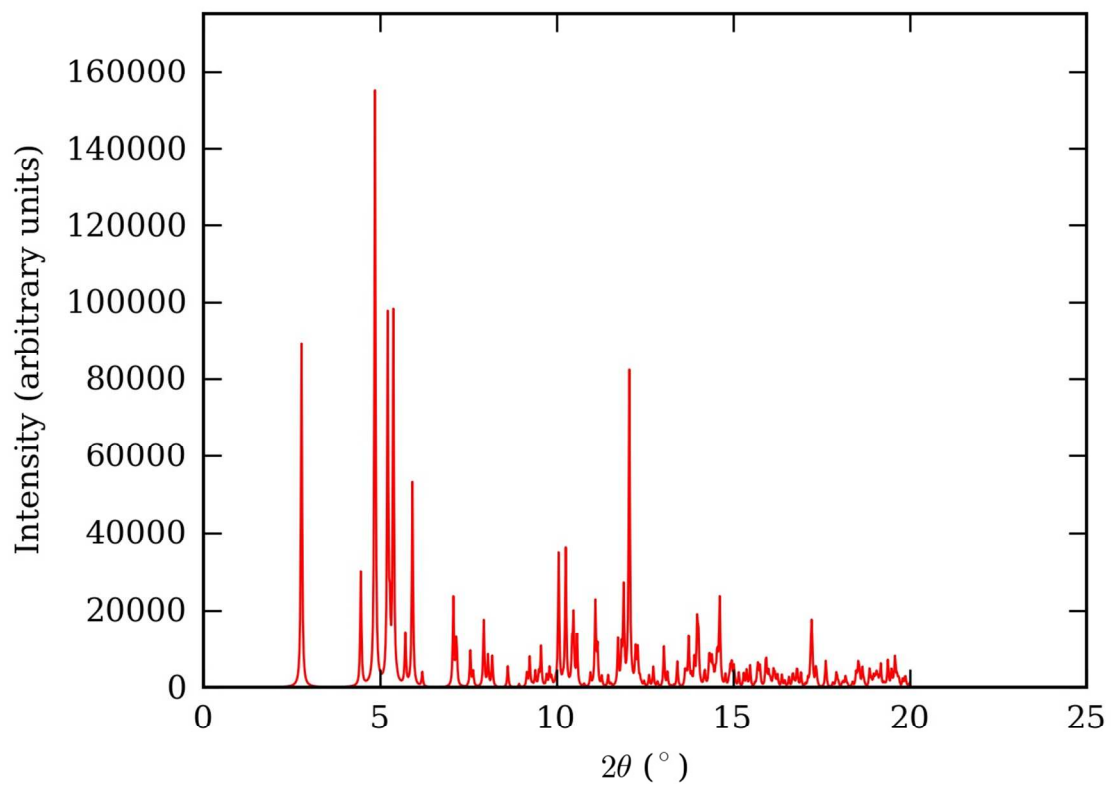


Figure S9 Powder X-ray diffraction patterns for complex **1**.

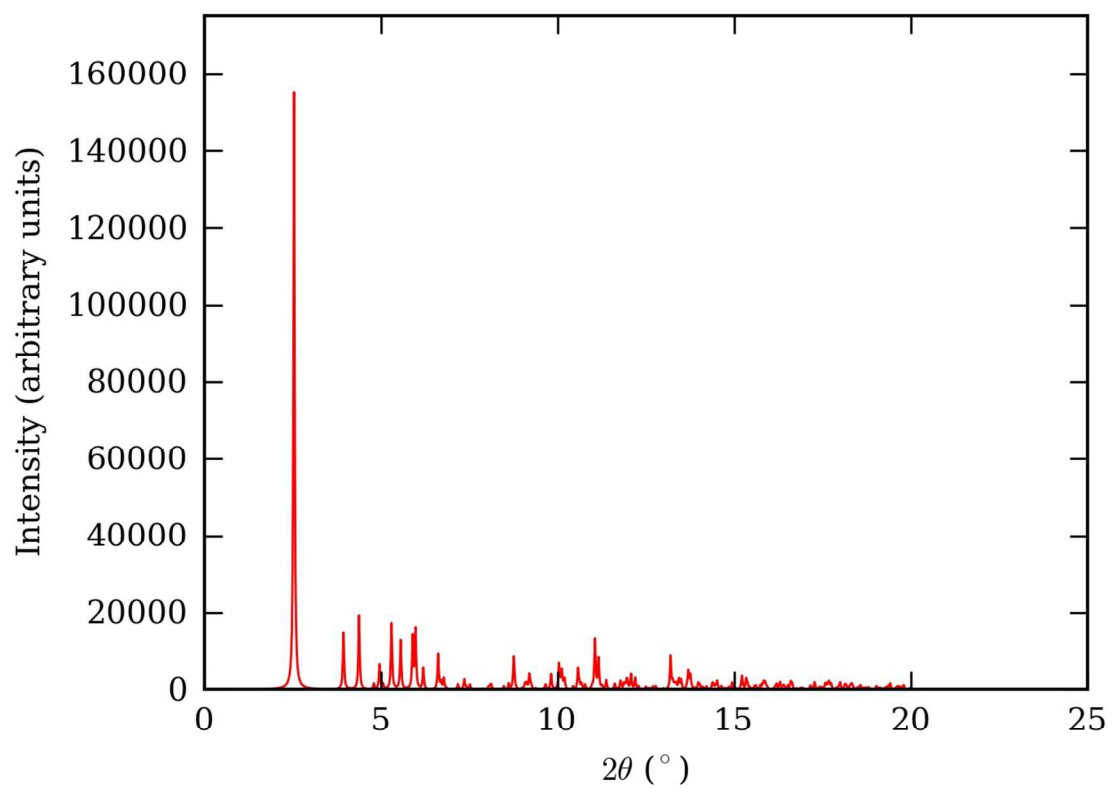


Figure S10 Powder X-ray diffraction patterns for complex **2**.

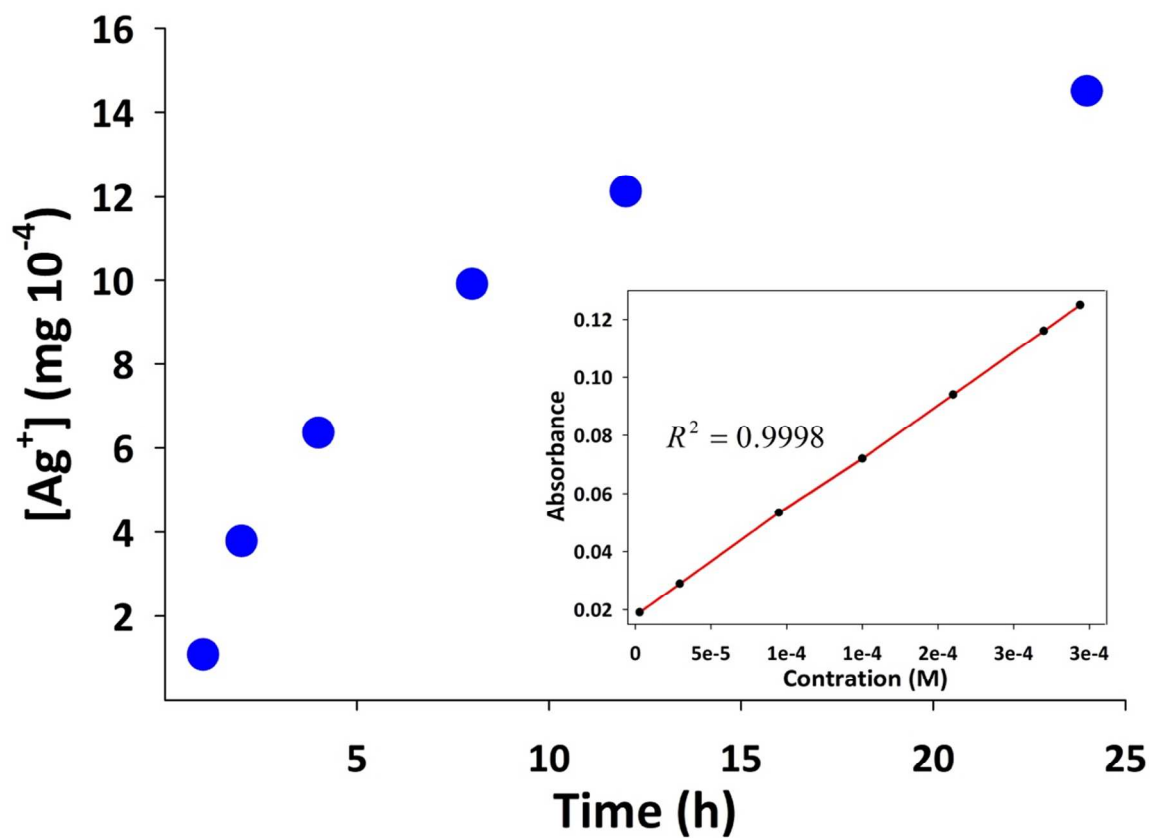


Figure S11 Leaching of Ag^+ from the silver-agar composite material in water analyzed by flame atomic absorption spectrophotometry

S. aureus

Resistant - not tested because >99% resistant

<i>Amp / Pen</i>	Not Specified	
Cefazolin	<=2 mcg/mL	Susceptible ¹
Clindamycin	<=0.5 mcg/mL	Susceptible ¹
Daptomycin	<=1 mcg/mL	Susceptible ²
Erythromycin	<=0.5 mcg/mL	Susceptible ³
Linezolid	2 mcg/mL	Susceptible ²
Minocycline	<=1 mcg/mL	Susceptible ²
Oxacillin	0.5 mcg/mL	Susceptible ³
Rifampin	<=0.5 mcg/mL	Susceptible ²
Tetracycline	<=0.5 mcg/mL	Susceptible ²
Trimethoprim/Sulfamethoxazole	<=0.5/9.5 m...	Susceptible ³
Vancomycin	1 mcg/mL	Susceptible ²

¹ HIGH risk of *C. diff* infection
² Low risk of *C. diff* infection
³ MODERATE risk of *C. diff* infection

and Collection

Figure S12 Sensitivity pattern for *S. aureus* clinical isolate obtained from UCSD Health

P. aeruginosa #1

Susceptibility		
	Pseudomonas aeruginosa Not Specified	
Amikacin	>32 mcg/mL	Resistant ¹
Aztreonam	>16 mcg/mL	Resistant ¹
Cefepime	>16 mcg/mL	Resistant ²
Ceftazidime	>16 mcg/mL	Resistant ²
Ciprofloxacin	>2 mcg/mL	Resistant ²
Colistin	1 mcg/mL	Susceptible ¹
Doripenem	>2 mcg/mL	Resistant ²
Gentamicin	>8 mcg/mL	Resistant ¹
Meropenem	>8 mcg/mL	Resistant ²
Piperacillin/Tazobactam	>64 mcg/mL	Resistant ³
Tobramycin	>8 mcg/mL	Resistant ¹
Trimethoprim/Sulfamethoxazole	>2/38 mcg/mL	Resistant ³
¹ Low risk of C. diff infection ² HIGH risk of C. diff infection ³ MODERATE risk of C. diff infection		

Susceptibility

Figure S13 Sensitivity pattern for *P. aeruginosa* 1 (P1) clinical isolate obtained from UCSD Health

Pseudo #2

Ph.D.

San Diego CA 92121

Susceptibility

	Pseudomonas aeruginosa (mucoid) Not Specified	
Amikacin	>32 mcg/mL	Resistant ¹
Aztreonam	>16 mcg/mL	Resistant ¹
Cefepime	>16 mcg/mL	Resistant ²
Ceftazidime	>16 mcg/mL	Resistant ²
Ciprofloxacin	2 mcg/mL	Intermediate ²
Doripenem	>2 mcg/mL	Resistant ²
Gentamicin	>8 mcg/mL	Resistant ¹
Meropenem	>8 mcg/mL	Resistant ²
Piperacillin/Tazobactam	>64 mcg/mL	Resistant ³
Tobramycin	8 mcg/mL	Intermediate ¹

¹ Low risk of C. diff infection

² HIGH risk of C. diff infection

³ MODERATE risk of C. diff infection

Figure S14 Sensitivity pattern for *P. aeruginosa* 2 (P2) clinical isolate obtained from UCSD Health

Figure S15. ESI-MS of complex 1

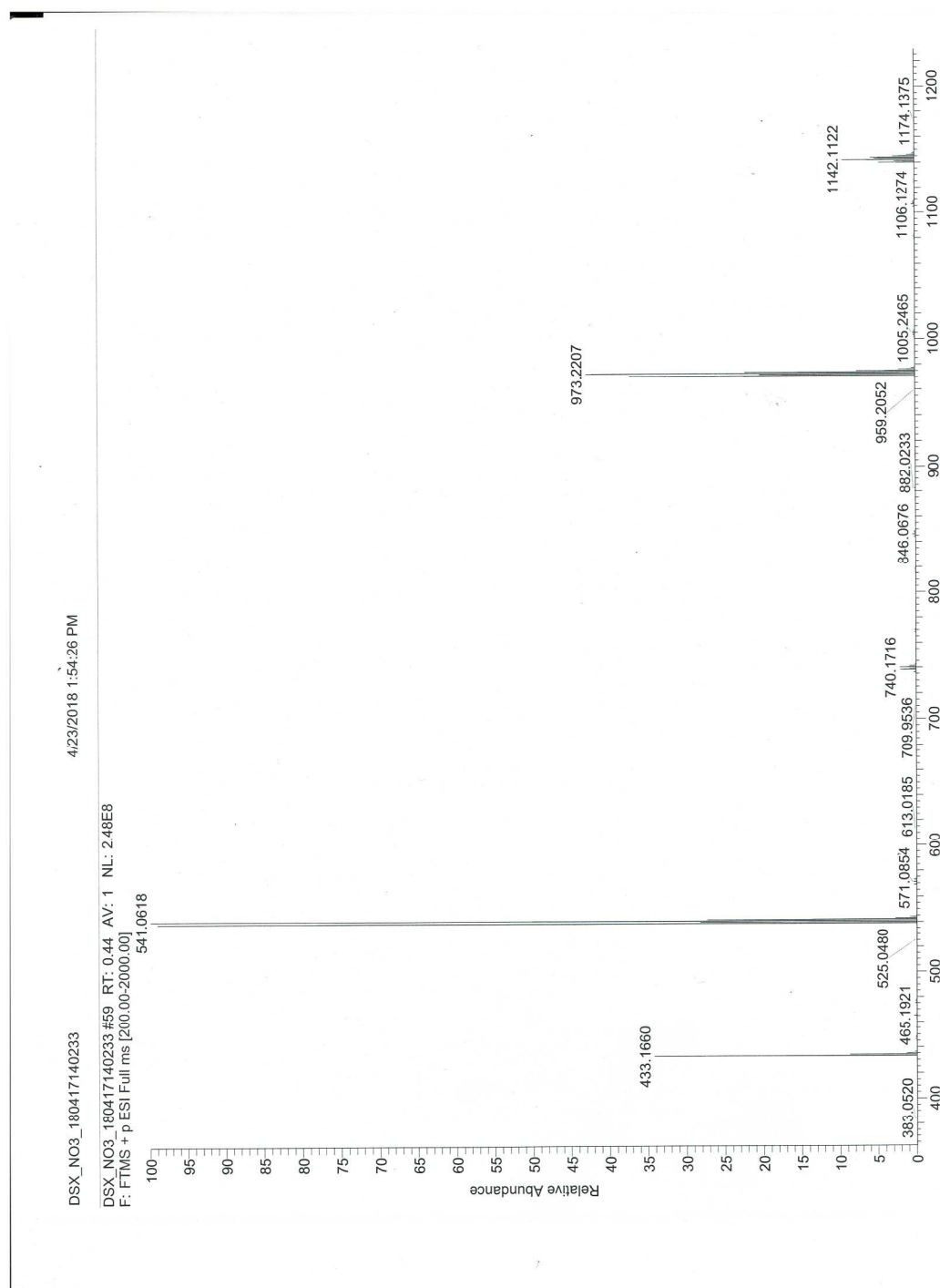
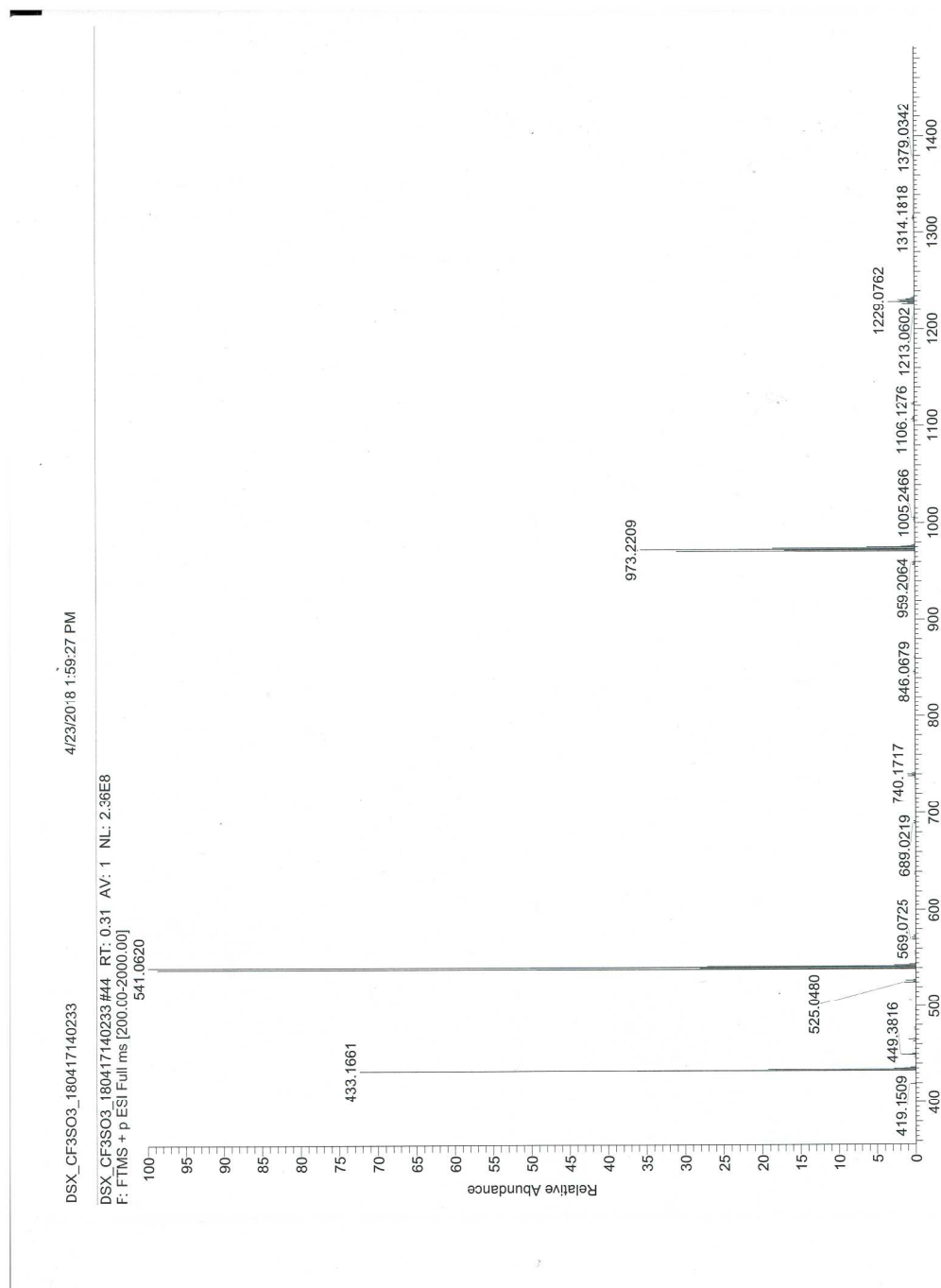


Figure S16. ESI-MS of complex 2



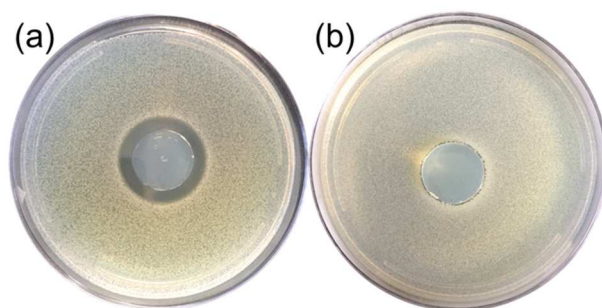


Figure S 17. Zones of inhibition upon incubation of *A. baumannii* with (a) complex1-agar disk and (b) ampicillin disk

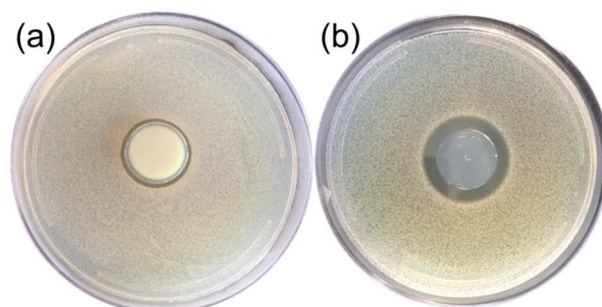


Figure S 18. Zones of inhibition produced by the agar composites containing (a) AgNO_3 , and (b) $[\text{Ag}_2(\text{DSX})_2(\text{NO}_3)_2]$ (**1**) on SSTI model inoculated with *A. baumannii*