Electronic Supplementary Information (ESI)

Hydrogels containing water soluble conjugates of silver(I) ions with amino acids, metabolites or natural products for non infectious contact lenses

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Description of the crystal structure of AGU

The structure of **AGU**, has been studied previously at room temperature [23] and in the present discussion an emphasis is given in the packing and the hydrogen bond interactions. Selected bond distances and angles are listed in Table AGU-1. **AGU** crystallizes in the monoclinic space group $P2_1/n$ and in asymmetric unit of the cell exist two Ag(I) cations, two NO_3^- anions and two urea molecules resulting in the chemical formula $Ag_2(NO_3)_2(CH_4N_2O)_2$, which is the repeating unit along the chains formed parallel to the c axis (Figure AGU-1). The nitrate groups bridge silver cations along the chains and the urea molecules are coordinated to silver atoms and occupy side positions along them and interact through hydrogen bonds with atoms belonging to neighboring chains (Table AGU-2) thus forming layers parallel to the (100) plane (Figure AGU-2a) and through the bonding of silver atoms with nitrogen atoms from urea molecules belonging to neighboring layers the 3D architecture of the structure is build (Figure AGU-2b). Ag1 cations is coordinated to five atoms (two oxygens form two nitrate group, one oxygen from an urea molecule lying at the side of the chain, and two nitrogen atoms from two urea molecules lying at neighboring layers) which form a trigonal bipyramid. The coordination polyhedron around the Ag2 cation is a trigonal pyramid, formed also by two oxygens form two nitrate groups, one oxygen from an urea molecule lying at the side of the chain but in this case only a nitrogen atoms from one urea molecule lying at neighboring layer is coordinated to it. All distances of N or O atoms which are coordinate to silver atoms are lying within the usually observed range range 2.339-2.489 Å, except from those of axial Ag1-N4 and Ag1-N3 which are a little longer.

Table AGU-1. Bond length (Å) and angles (°) for **AGU**.

Ag1—O8	2.3385 (18)	N2—O6	1.258 (3)
Ag1—O2	2.415 (2)	N2—O4	1.252 (3)
Ag1—O6	2.489 (2)	O7—C1	1.250 (3)
Ag2—O7	2.3423 (19)	C1—N4	1.347 (3)
Ag2—N5´´´	2.398 (3)	C1—N3	1.361 (3)
Ag2—O4*	2.455 (7)	C2—O8	1.241 (3)
Ag2—O3	2.453 (2)	C2—N6	1.336 (3)
N1—O1	1.228 (3)	C2—N5	1.380 (3)
N1—O2	1.257 (3)	Ag1—N4´	2.682(2)
N1—O3	1.251 (3)	Ag1—N3´´	2.648(3)
N2—O5	1.243 (3)		
O8—Ag1—O2	130.66 (7)	O5—N2—O6	120.3 (2)
O8—Ag1—O6	97.25 (6)	O5—N2—O4	120.4 (2)
O2—Ag1—O6	131.29 (7)	O6—N2—O4	119.2 (2)
O7—Ag2—N5´´´	129.27 (7)	N2—O4—Ag2***	105.0 (2)
O7—Ag2—O4*	124.42 (7)	N2—O6—Ag1	104.7 (2)
N5i—Ag2—O4*	87.20 (8)	C1—O7—Ag2	123.5 (2)
O7—Ag2—O3	89.88 (7)	O7—C1—N4	121.2 (2)
N5i—Ag2—O3	116.0 (3)	O7—C1—N3	121.6 (2)
O4ii—Ag2—O3	116.55 (8)	N4—C1—N3	117.2 (2)
O1—N1—O2	120.4 (2)	O8—C2—N6	123.7 (3)
O1—N1—O3	120.7 (2)	O8—C2—N5	120.5 (2)
O2—N1—O3	118.9 (2)	N6—C2—N5	115.9 (2)
N1—O2—Ag1	107.0 (2)	C2—O8—Ag1	127.8 (2)
N1—O3—Ag2	113.1 (2)	C2—N5—Ag2**	110.3 (2)

Symmetry codes: (´):2-x,1-y,1-z;(´´):1-x,1-y,1-z; (´´´) *x*-1/2, -*y*+1/2, *z*-1/2; (*) *x*, *y*, *z*-1; (**) *x*+1/2, -*y*+1/2, *z*+1/2; (***) *x*, *y*, *z*+1;

Table AGU-2. Hydrogen bond geometry parameters (Å, º) for **AGU**.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
Intrachain Hydrogen bonds				
N3—H3*A*···O3	0.82 (4)	2.15 (4)	2.961 (3)	171 (3)
N6—H6*A*···O6	0.80 (4)	2.39 (4)	3.093 (3)	147 (4)
Interchain Hydrogen bonds				
N3—H3*B*···N2^{v}	0.83 (4)	2.65 (4)	3.459 (3)	165 (3)
N3—H3*B*···O4^{v}	0.83 (4)	2.44 (3)	3.136 (3)	141 (3)
N3—H3*B*···O6^{v}	0.83 (4)	2.17 (4)	2.975 (3)	162 (3)
N4—H4*A*···O8^{vi}	0.81 (4)	2.18 (4)	2.972 (3)	165 (3)
N4—H4*B*···O1^{vi}	0.82 (4)	2.61 (4)	3.074 (3)	118 (3)
N4—H4*B*···O4^{v}	0.82 (4)	2.26 (4)	3.024 (3)	155 (3)
N5—H5*A*···O7^{vii}	0.80 (4)	2.14 (4)	2.931 (3)	175 (3)
N5—H5*B*···O2^{viii}	0.85 (4)	2.45 (4)	3.070 (3)	130 (3)
N5—H5*B*···O5^{viii}	0.85 (4)	2.62 (3)	2.964 (3)	106 (3)
N6—H6*B*···O2^{viii}	0.90 (4)	2.29 (4)	3.114 (3)	152 (3)
N6—H6*B*···O3^{viii}	0.90 (4)	2.51 (4)	3.284 (3)	145 (3)

Symmetry codes: (v) -*x*+3/2, *y*+1/2, -*z*+3/2; (vi) -*x*+3/2, *y*+1/2, -*z*+1/2; (vii) -*x*+3/2, *y*-1/2, -*z*+1/2; (viii) -*x*+3/2, *y*-1/2, -*z*+3/2.

Table AGU-3. Crystallographic data for **AGU**

	1
Formula	$[CH_4AgN_3O_4]_n$
Fw	459.88
Space group	*P* $2_1/n$
a (Å)	6.2509(1)
b (Å)	16.8667(4)
c (Å)	10.2467(3)
β (º)	102.191(1)
V (Å^3)	1055.97(4)
Z	4
T (ºC)	-93
Radiation	Mo Kα
ρ_{calcd} (g cm^{-3})	2.893
μ (mm^{-1})	3.760
Reflections with $I>2\sigma(I)$	2149
R_1[a]	0.0212
wR_2[a]	0.0469

[a] $R_1 = \Sigma(||F_o|-|F_c||)/\Sigma(|F_o|)$ and $wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.
$w=1/[\sigma^2(F_o^2) +(\alpha P)^2+bP]$ and $P = [\max(F_o^2,0) +2F_c^2]/3$, a = 0.0129, b = 1.9062 for **AGU**,

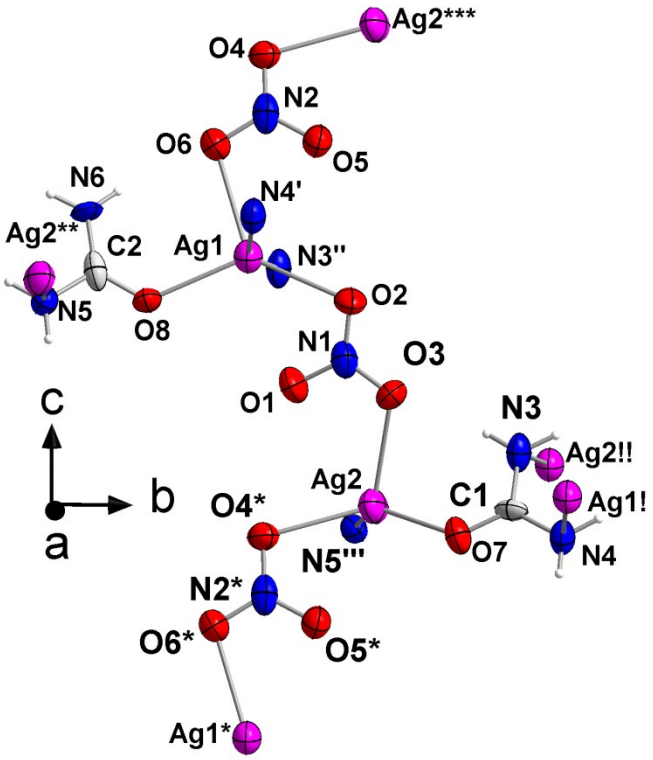
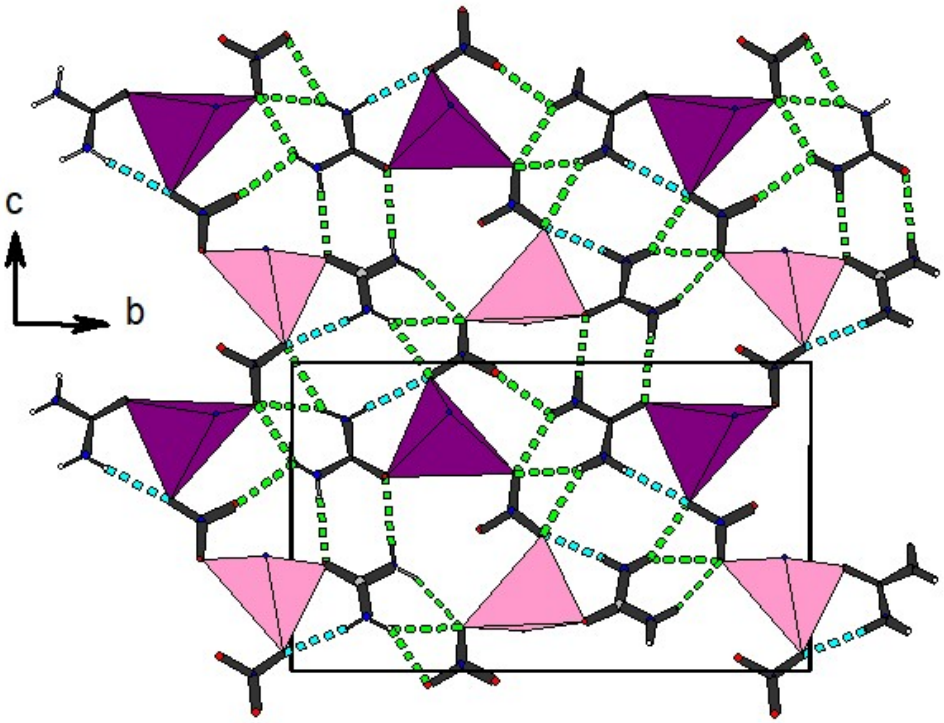
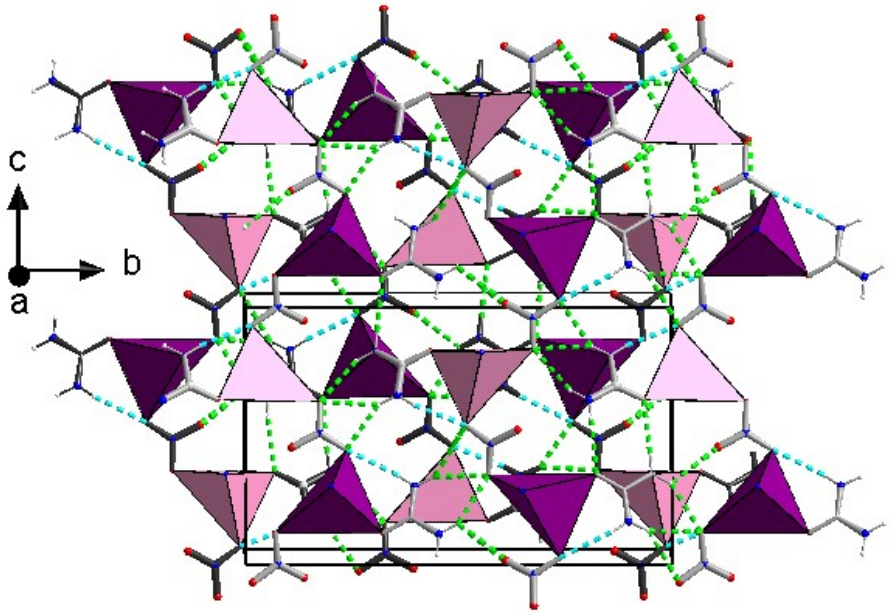


Figure AGU-1. Ortep type partial labeled molecular plot for **AGU.** Symmetry code: (´):2-x,1-y,1-z; (´´):1-x,1-y,1-z; (´´´):-0.5+x,0.5-y,-0.5+z; (*):x,y,-1+z; (**):0.5+x,0.5-y,0.5+z,x,y,1+z. White small spheres represent Hydrogen atoms.



(a)



(a)

Figure AGU-2. (a) Layers formed parallel to the (100) plane. Dashed thick cyan and light green lines indicate intrachain and interchain N-H···O hydrogen bonds respectively. (b) Relative position of two successive layers stacked along a axis. The bonds at the top layer are indicated with light grey color. Dark violet and pink polyhedral represent the polyhedra formed around Ag1 (trigona bipyramid) and Ag2 (trigonal pyramid) respectively.

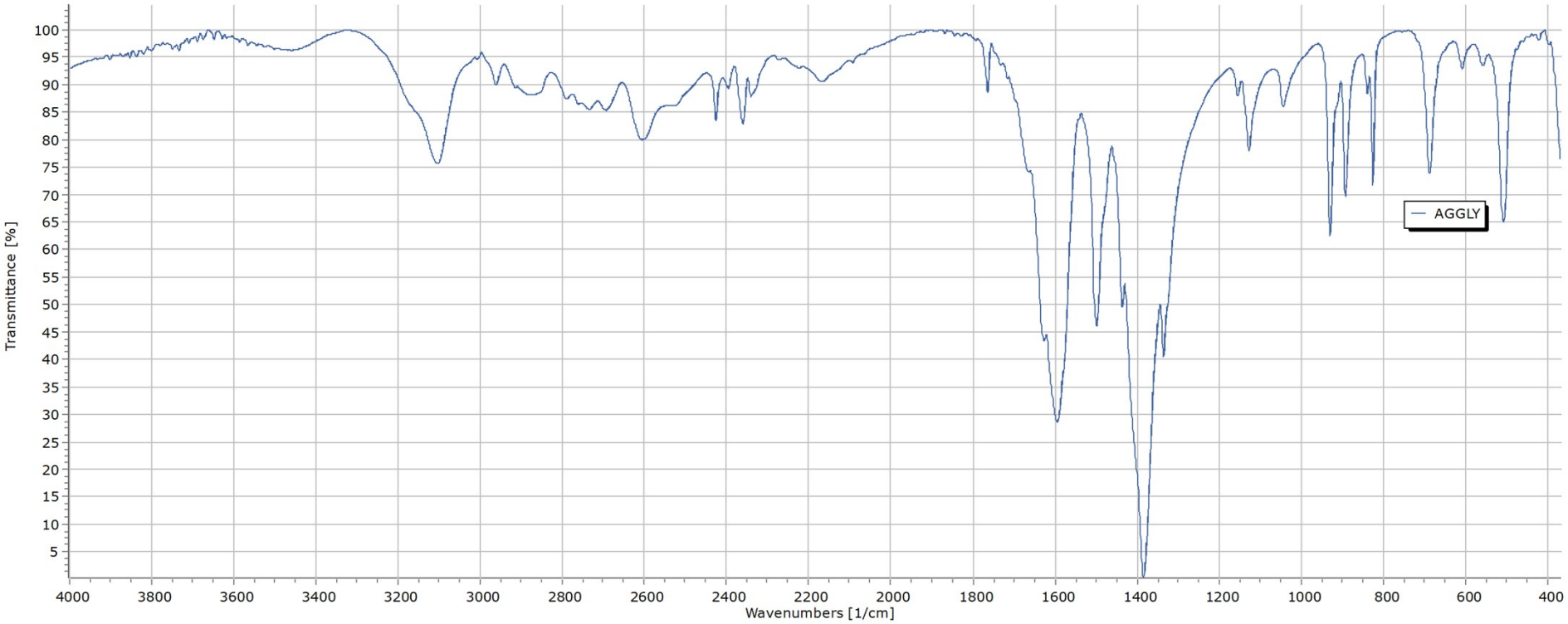


Figure S1. ATR-FT-IR spectrum of **AGGLY**

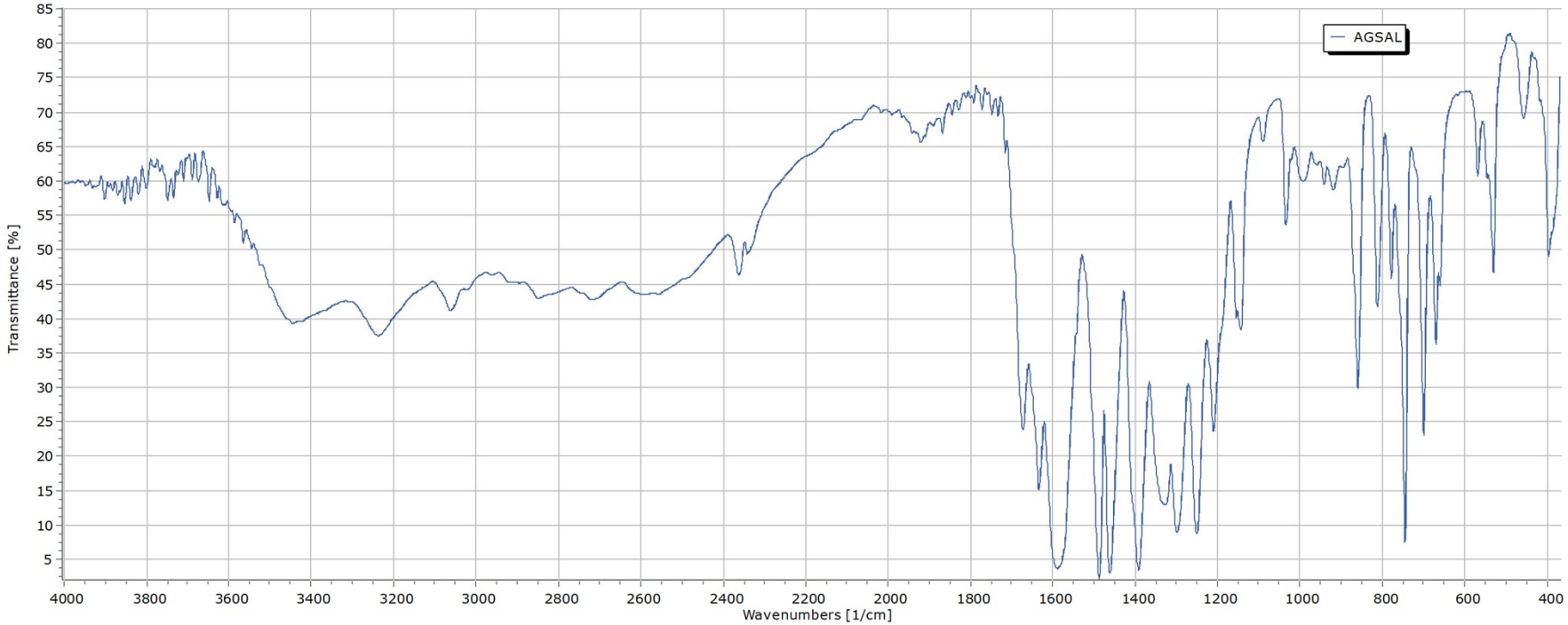


Figure S2. . ATR-FT-IRspectrum of **AGSAL**

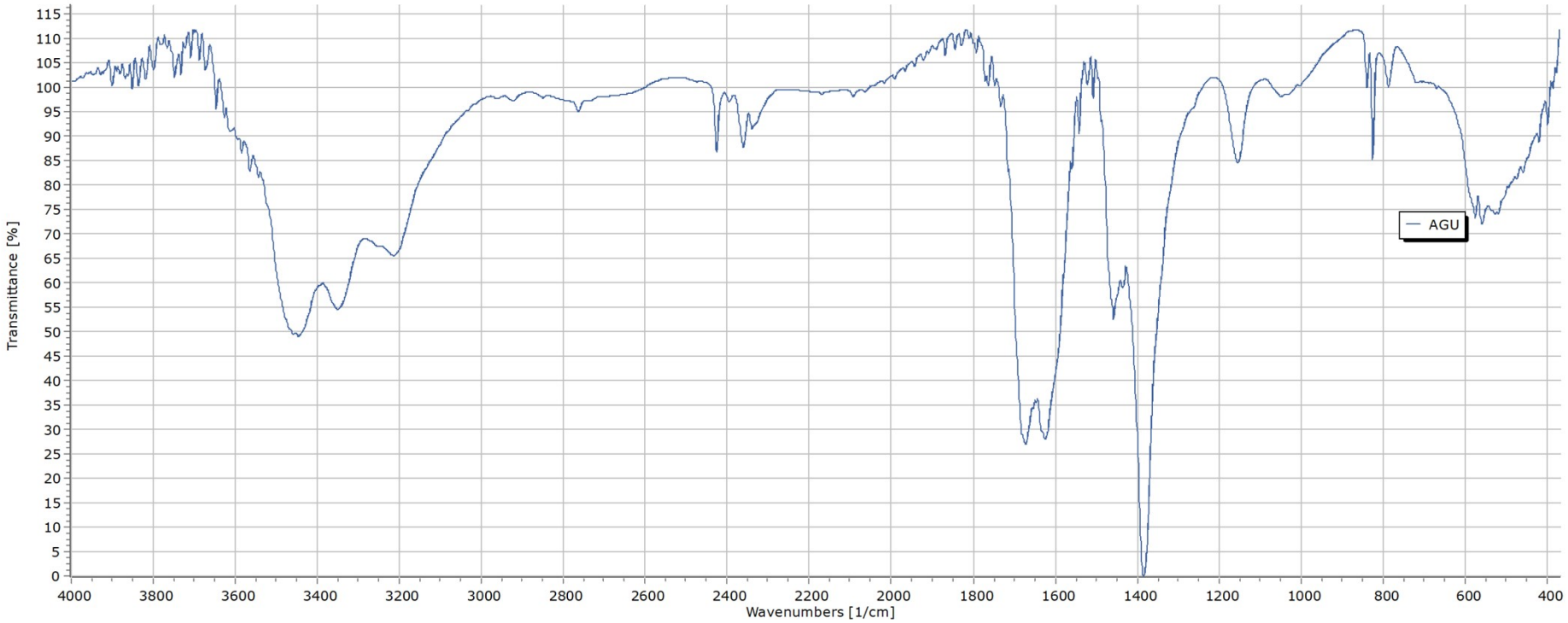


Figure S3. ATR-FT-IRspectrum of **AGU**.

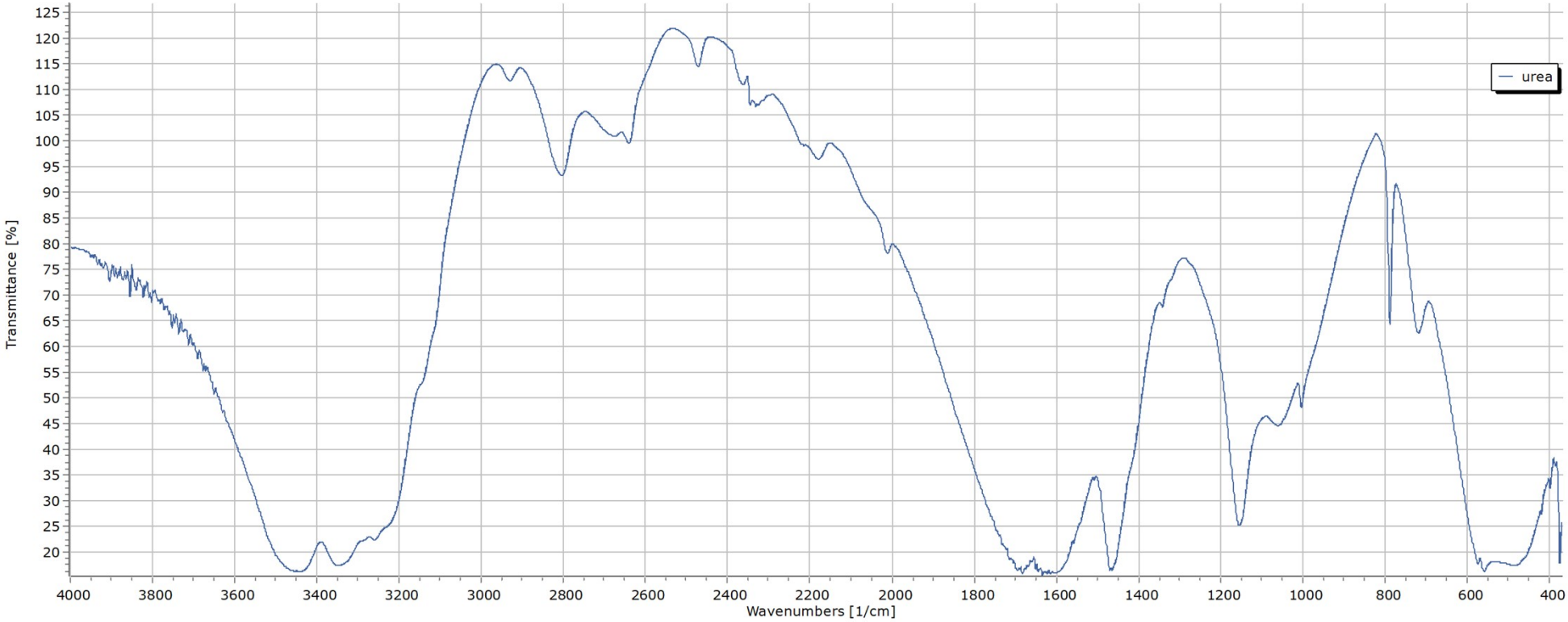


Figure S4. . ATR-FT-IR spectrum of U.

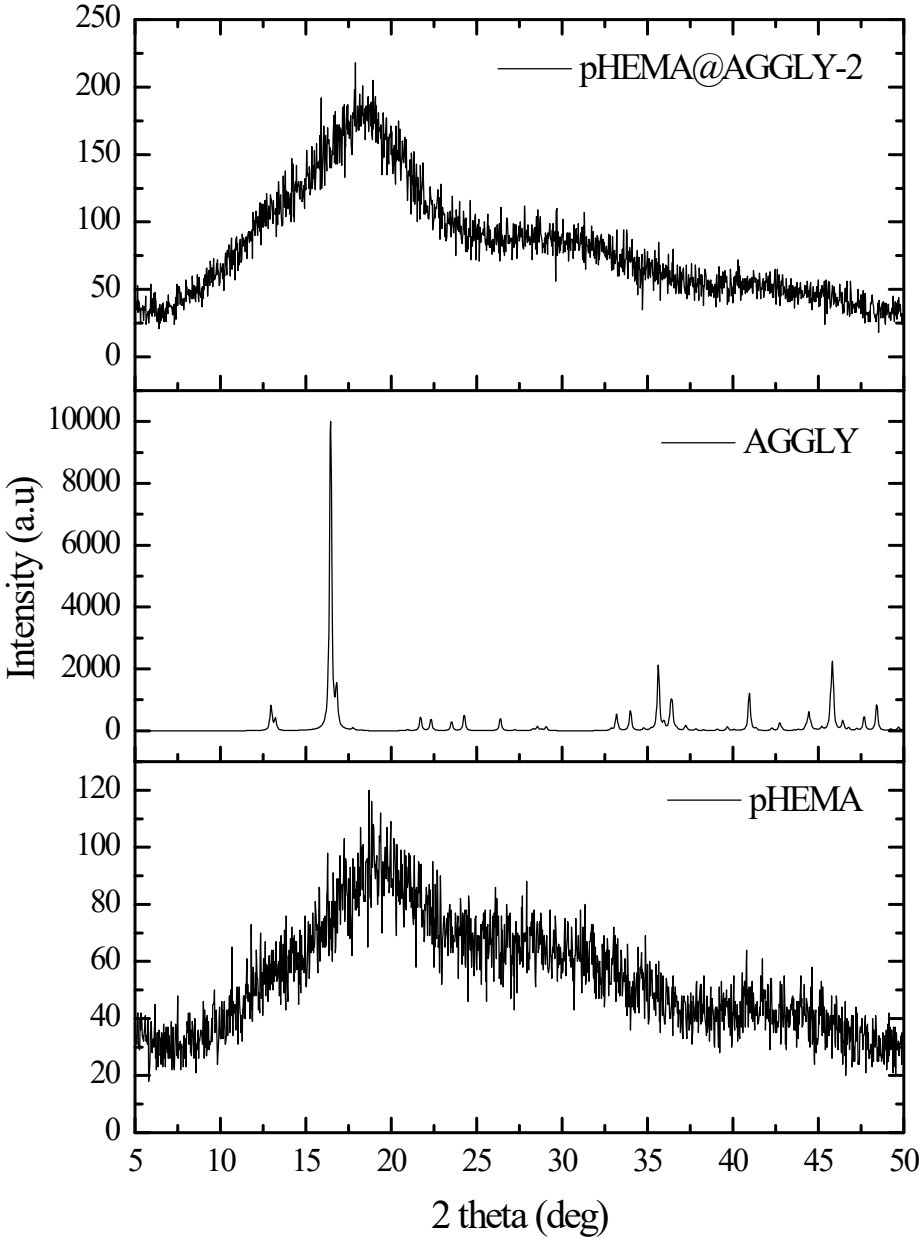


Figure S5. Powder X-ray diffraction diagram of **pHEMA@AGGLY-2** against the corresponding of pHEMA and the one of **AGGLY** calculated from single crystal diffraction data

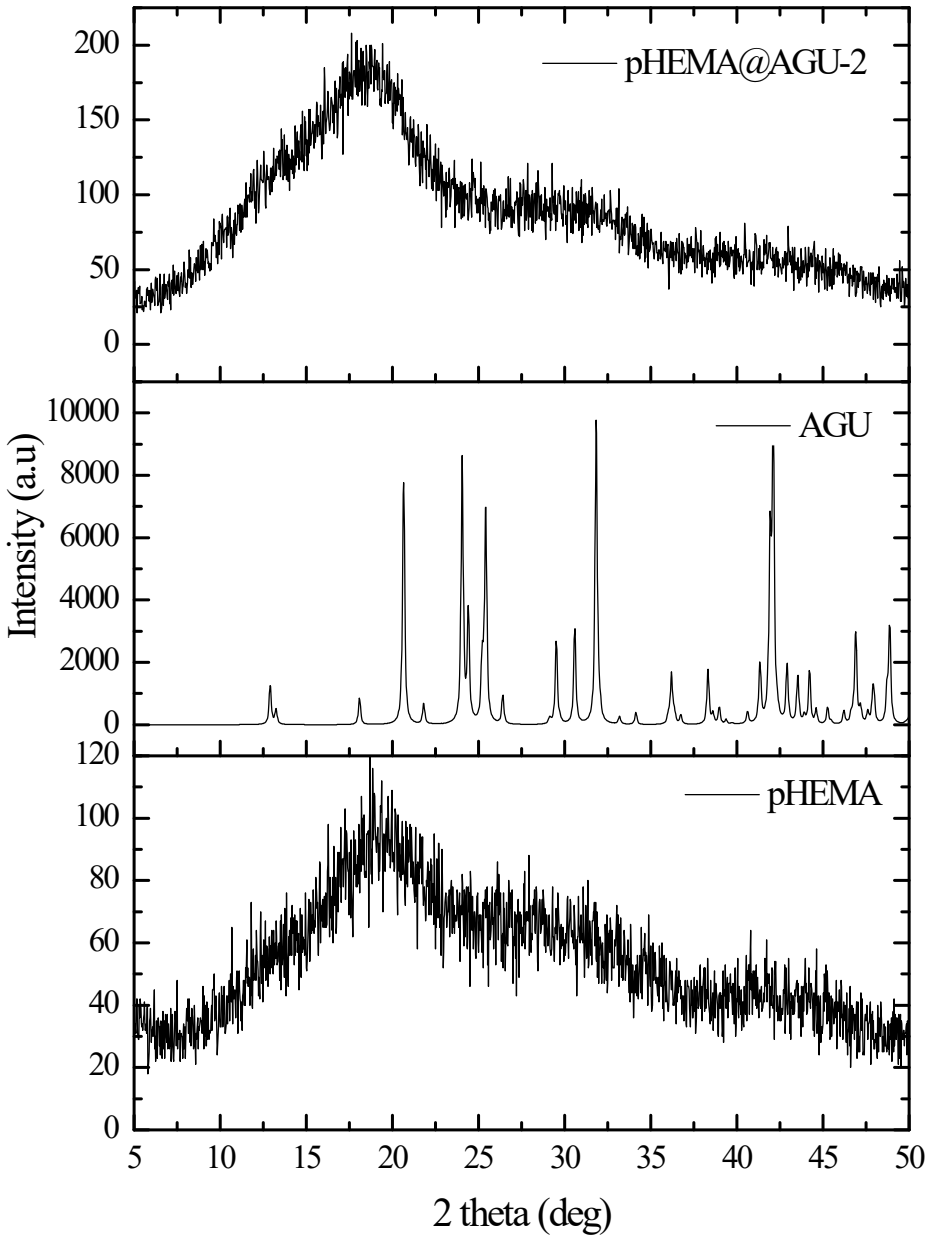


Figure S6. Powder X-ray diffraction diagram of **pHEMA@AGU-2** against the corresponding of pHEMA and the one of **AGU** calculated from single crystal diffraction data

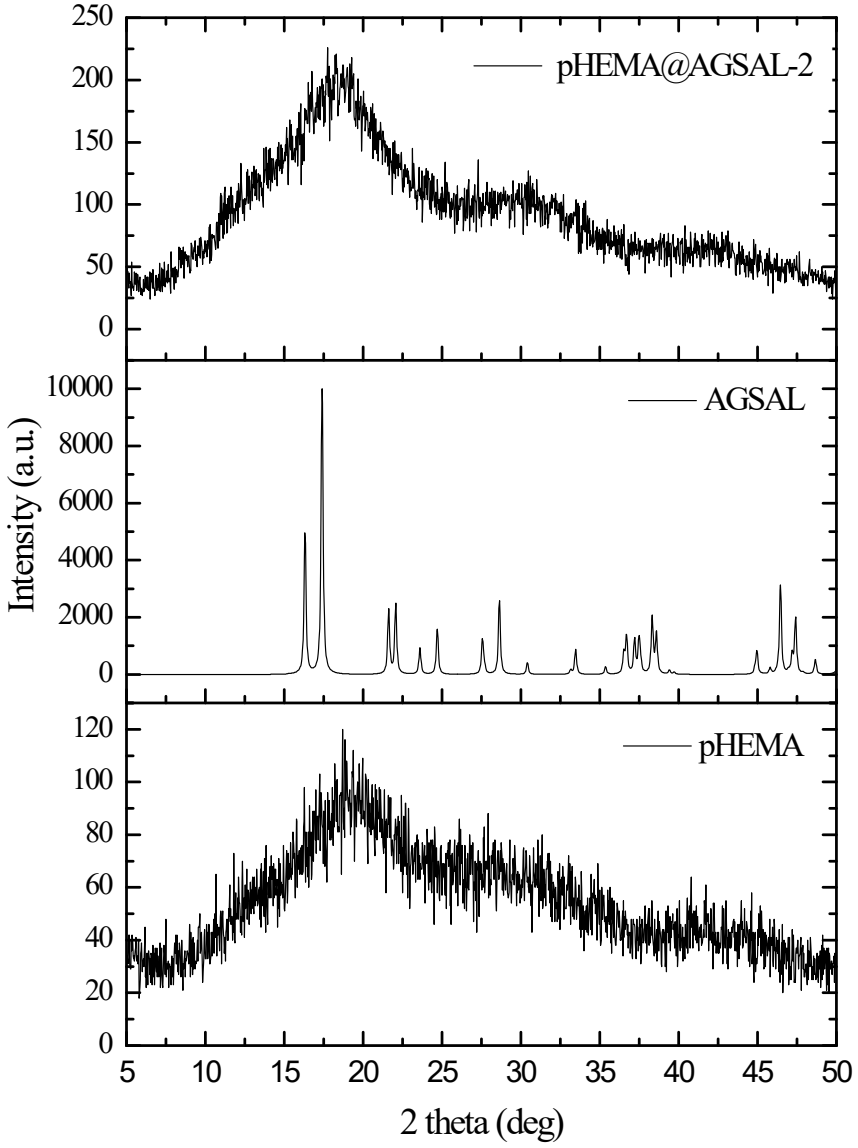


Figure S7. Powder X-ray diffraction diagram of **pHEMA@AGSAL-2** against the corresponding of pHEMA and the one of **AGSAL** calculated from single crystal diffraction data

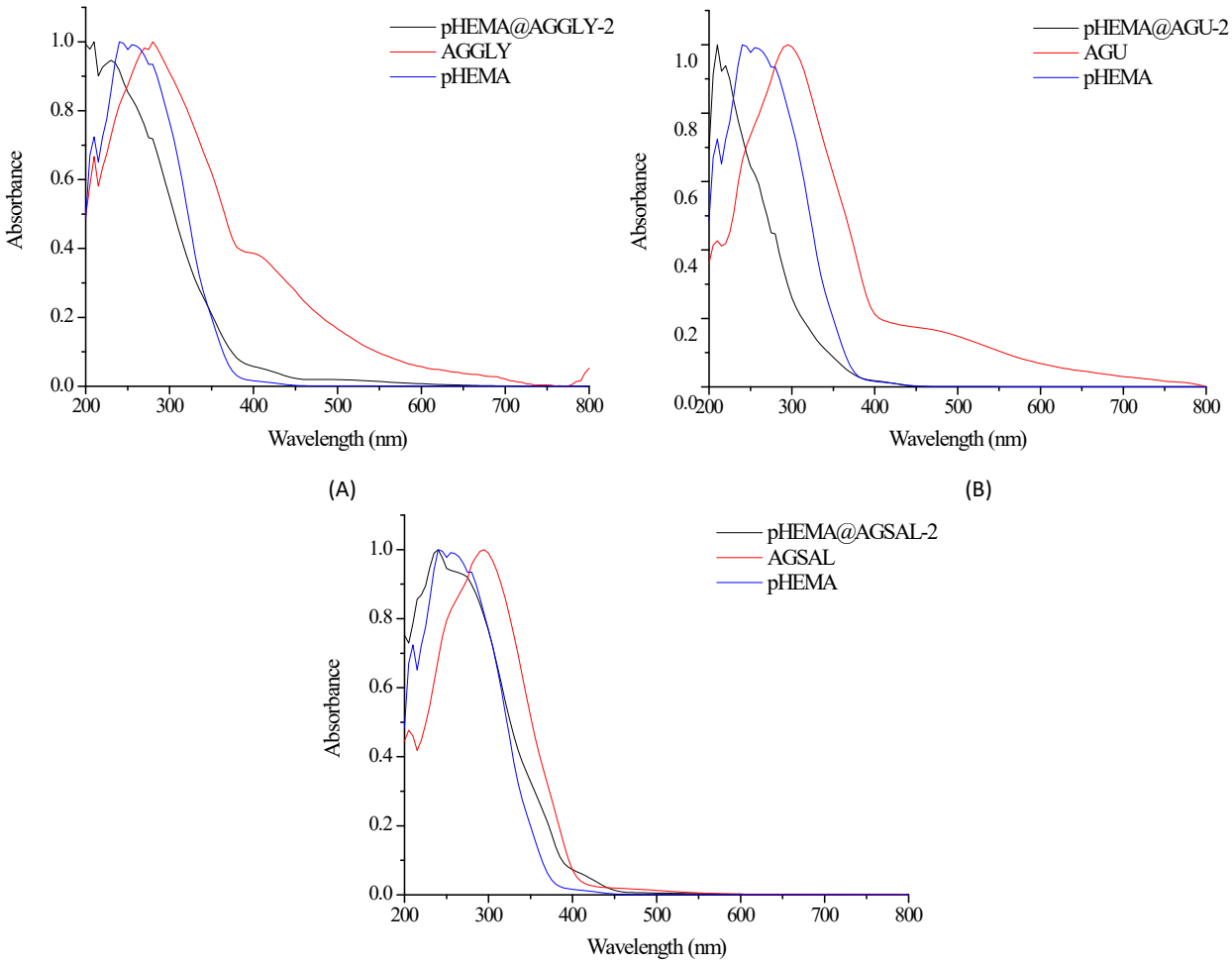
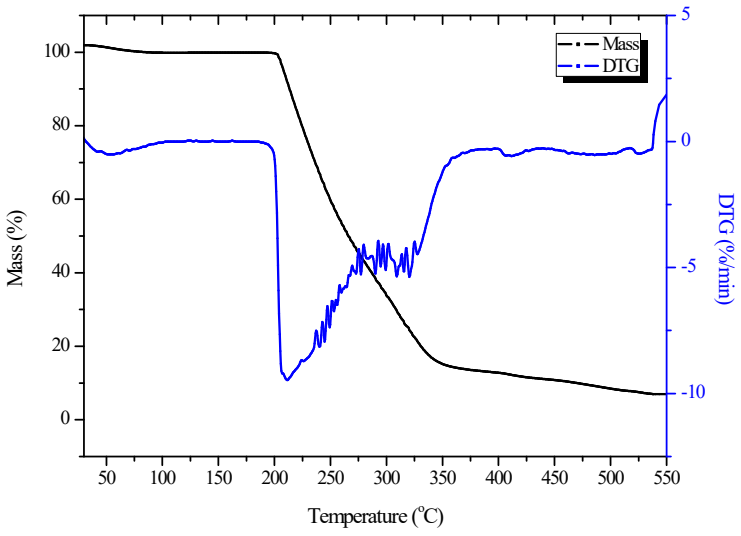
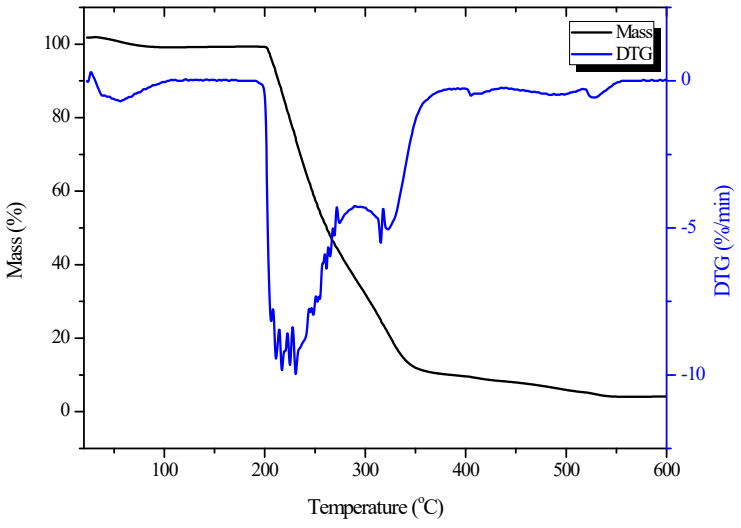


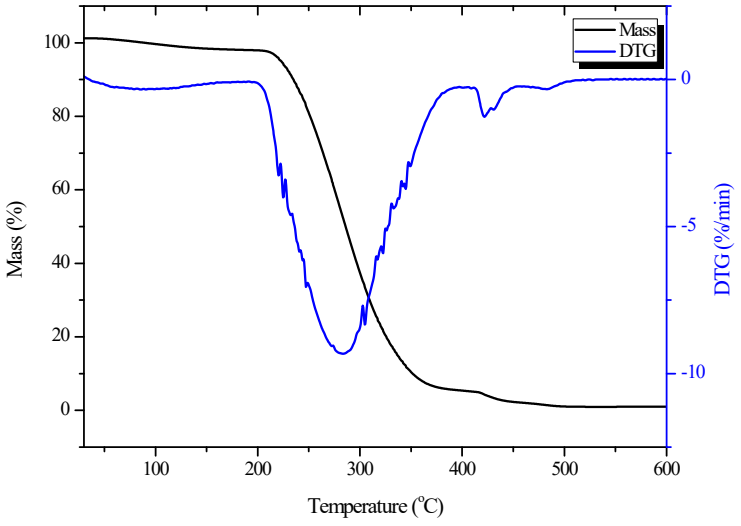
Figure S8. UV-Vis DRS of pHEMA, **pHEMA@AGGLY-2**, **AGGLY** (A), **pHEMA@AGU-2**, **AGU** (B) and **pHEMA@AGSAL-2**, **AGSAL** (C)



(A)

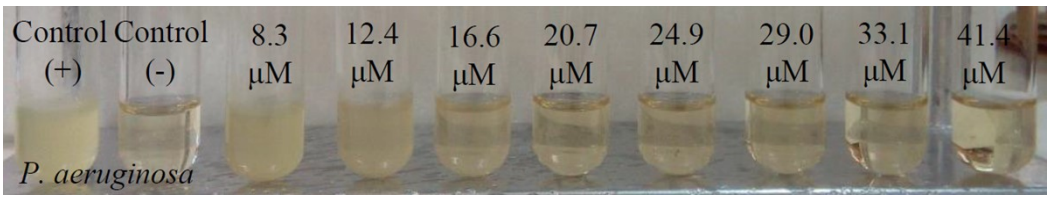


(B)

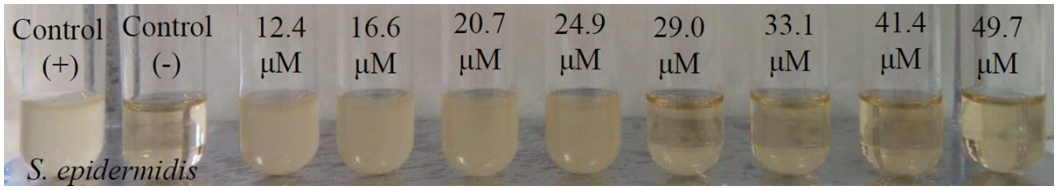


(C)

Figure S9. TGA diagrams of **pHEMA@AGGLY-2** (A), **pHEMA@AGU-2** (B) and **pHEMA@AGSAL-2** (C)



(A)



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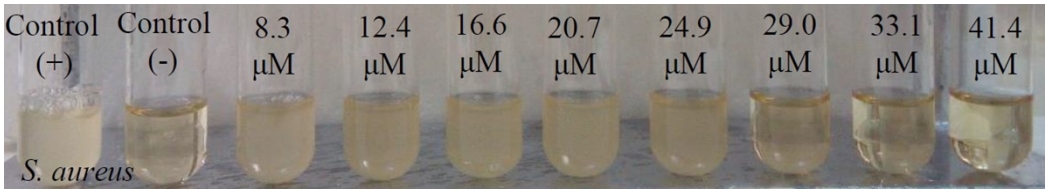
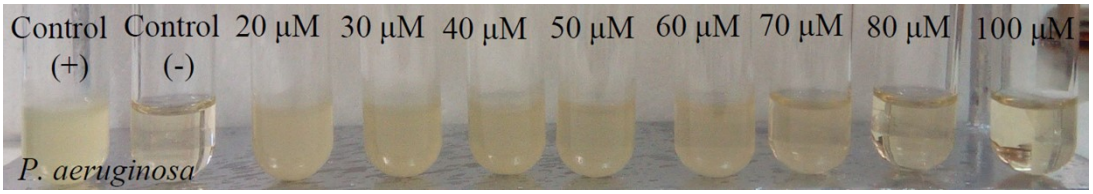
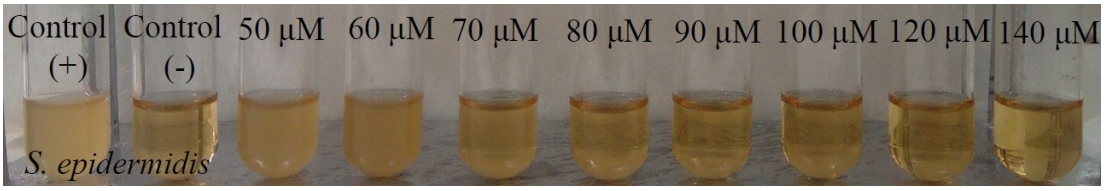


(C)

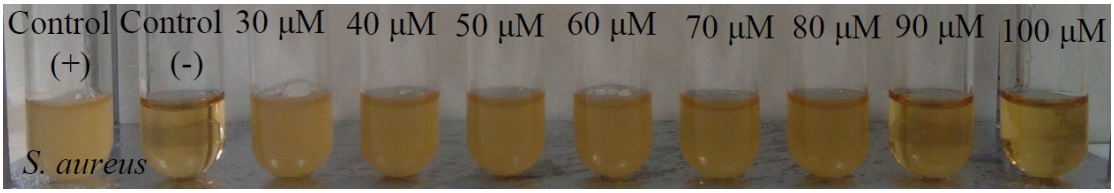
Figure S10. Minimum Inhibitory Concentration of **AGGLY** against *P. aeruginosa* (A), *S. epidermidis* (B) and *S. aureus* (C)



(A)

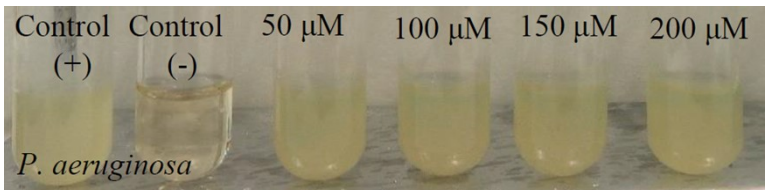


(B)

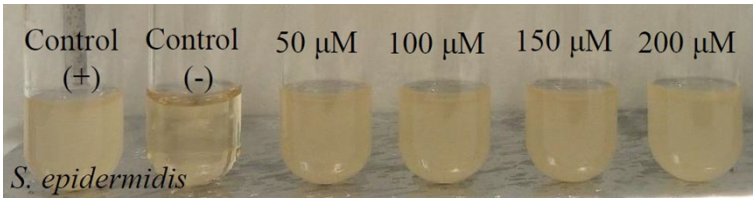


(C)

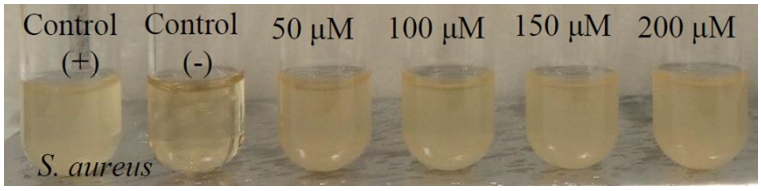
Figure S11. Minimum Inhibitory Concentration of **AGU** against *P. aeruginosa* (A), *S. epidermidis* (B) and *S. aureus* (C)



(A)

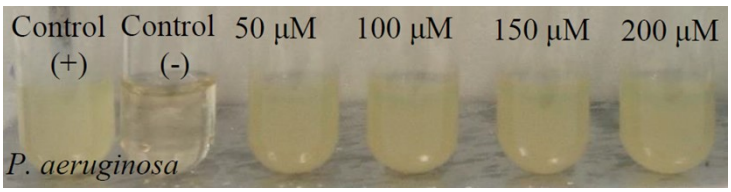


(B)

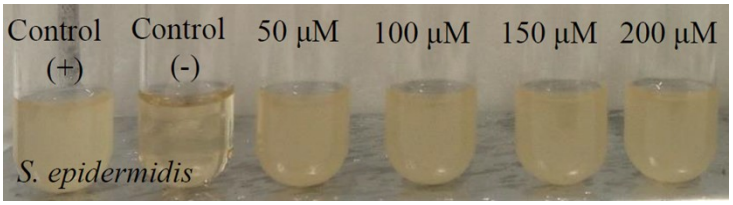


(C)

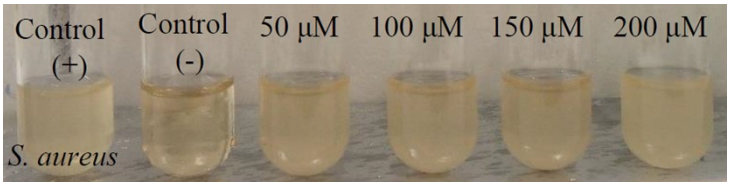
Figure S12. Minimum Inhibitory Concentration of GlyH against *P. aeruginosa* (A), *S. epidermidis* (B) and *S. aureus* (C)



(A)

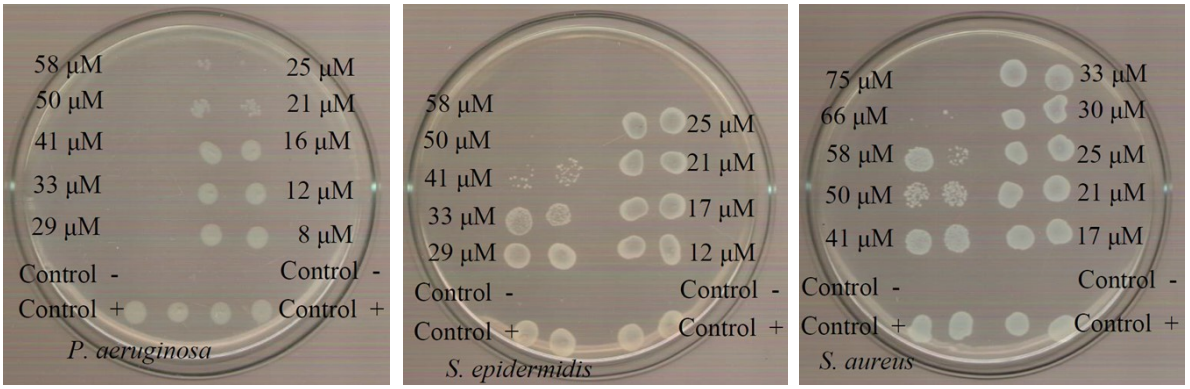


(B)

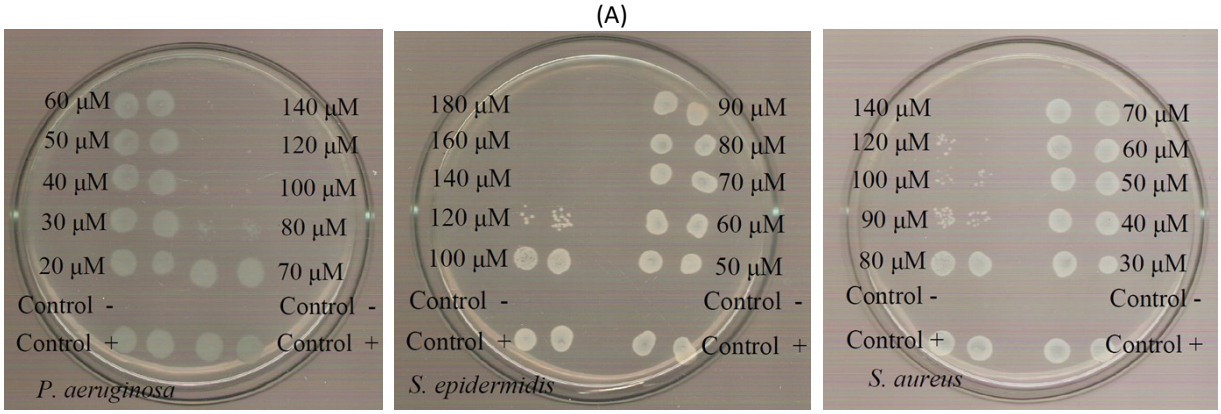


(C)

Figure S13. Minimum Inhibitory Concentration of urea against *P. aeruginosa* (A), *S. epidermidis* (B) and *S. aureus* (C)

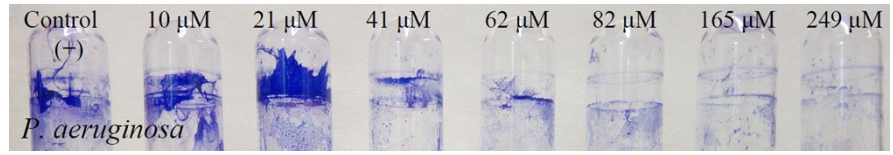


(A)

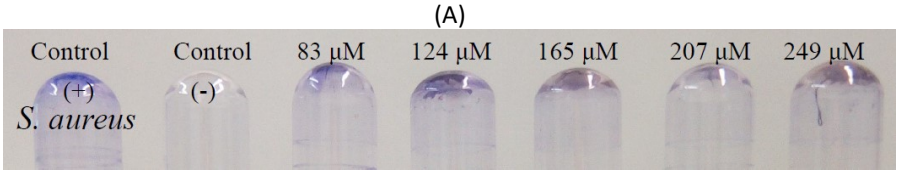


(B)

Figure S14. Minimum bactericidal concentration of **AGGLY** (A) and **AGU** (B) against *P. aeruginosa, S. epidermidis* and *S. aureus*



(A)



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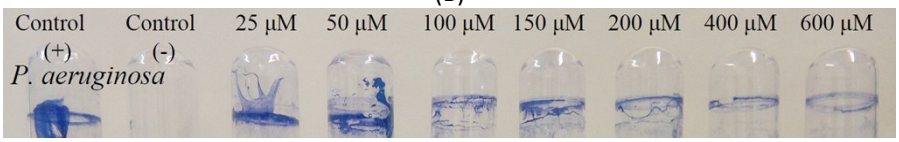
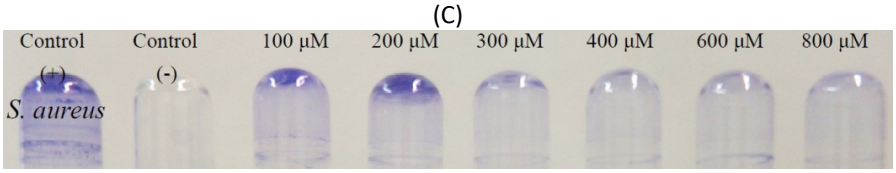


(C)



(D)

Figure S15. *P. aeruginosa* (A, C) and *S. aureus* (B, D) biofilms stained by crystal violet under increasing concentrations of **AGGLY** (A, B) and **AGU** (C, D)