

## *Supporting information for*

# **Molecular Dynamics and Docking Simulations in Exploring a Potential Extracellular Matrix-Based Antibiofilm: Fighting the Resistant *Pseudomonas aeruginosa*-*Candida albicans***

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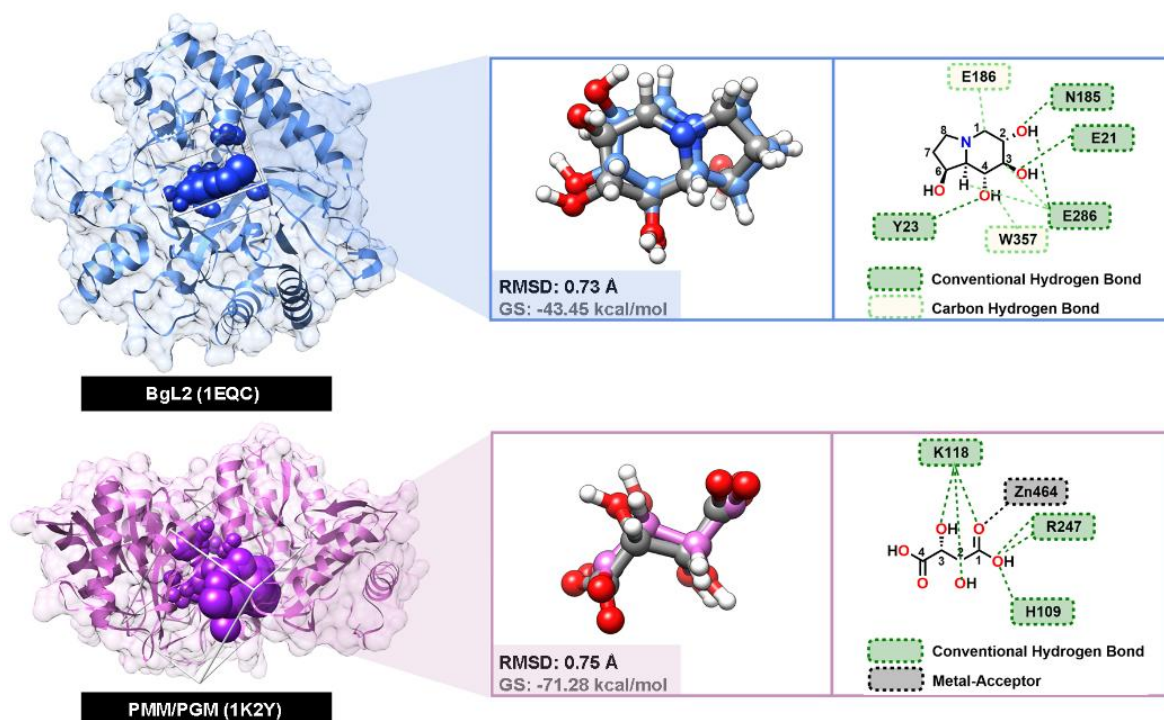
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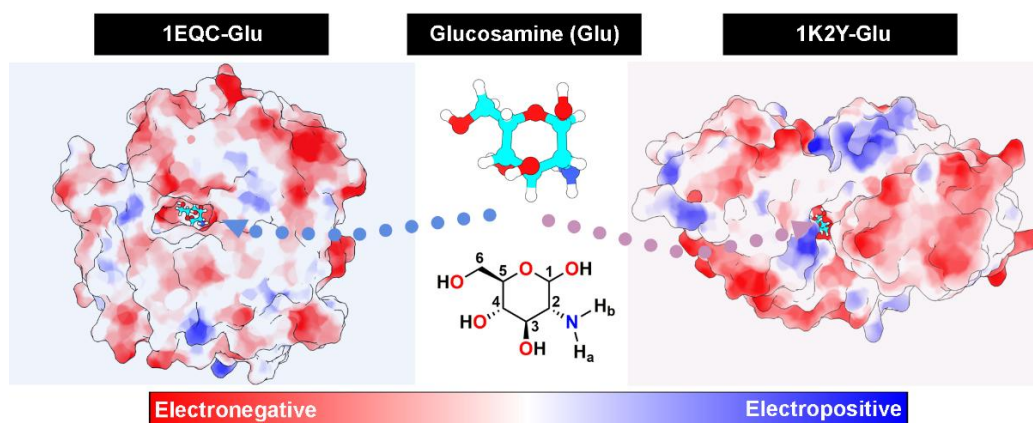
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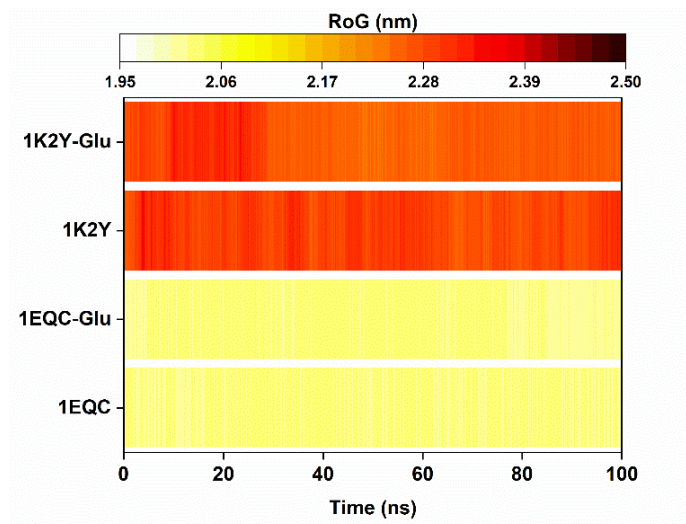
DOI: <http://dx.doi.org/10.30919/es1386>



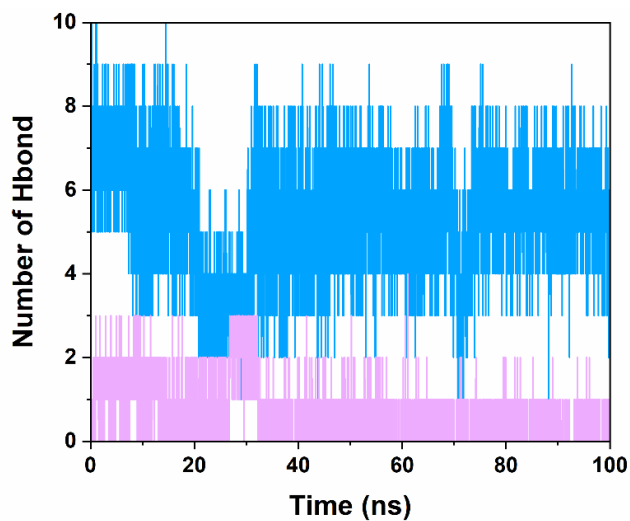
**Fig. S1:** Redocking step: selected sphere and grid box. The superposition of native ligands is shown by redocking pose (blue and orchid) and co-crystal (gray).



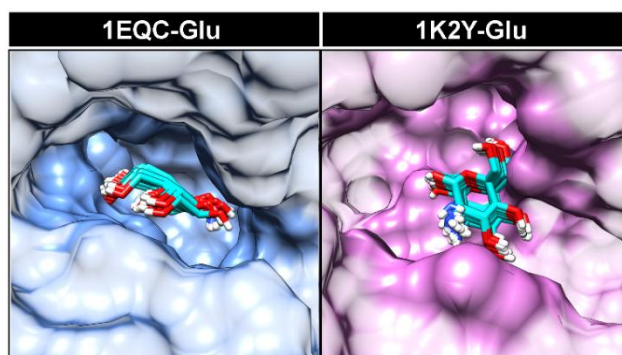
**Fig. S2:** Molecular docking of glucosamine into BgL2 and PMM/PGM. The coulombic surface is shown by the range color red (the most electronegative) to blue (the most electropositive).



**Fig. S3:** System rigidity is performed by the radius of gyration (RoG) along 100 ns simulation time. The lowest to highest fluctuation is colored from white to black.



**Fig. S4:** The number of hydrogen bonds is recorded along 100 ns of simulation.



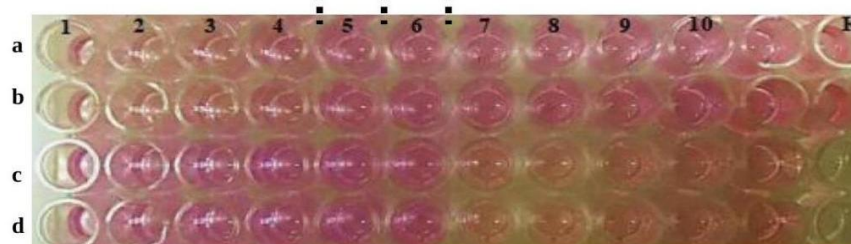
**Fig. S5:** The Glu superposition (20 snapshots) on the pocket site of the targeted protein was extracted using the last 20 ns of trajectories.

Antibiotics	Well numbers in microtiterplate							
	1	2	3	4	5	6	7	8
Meropenem (µg/mL)	8.000	4.000	2.000	1.000	0.500	0.250	0.125	0.063
Fluconazole (µg/mL)	1.000	0.500	0.250	0.125	0.063	0.031	0,016	0.008



**Fig. S6:** Determination of the MIC of a single antibiotic in a 96-well microtiter plate. Rows a and b: meropenem. Rows c and d: fluconazole. Columns 1-8: well numbers. C1, C2, and C3: controls for antimicrobials, solvent, and cell growth, respectively.

Experiments		Well numbers in microtiterplate									
		1	2	3	4	5	6	7	8	9	10
B1	[Meropenem] (mg/mL)	8.000	4.000	2.000	1.000	0.500	0.250	0.1250	0.062	0.031	0.015
	[Flukonazol] (mg/mL)	0,125	0,125	0,125	0,125	0,125	0,125	0,125	0,125	0,125	0,125
B2	[Flukonazol] (mg/mL)	0.500	0.250	0.125	0.062	0.031	0,016	0.008	0.004	0.002	0.001
	[Meropenem] (mg/mL)	0,500	0,500	0,500	0,500	0,500	0,500	0,500	0,500	0,500	0,500



**Fig. S7:** Determination of the MICs of antibiotic combinations in a 96-well microtiter plate. B1 and B2 were the experiments used to determine the MICs of meropenem and fluconazole, respectively. Rows a and b: experiment B1, rows c and d: experiment B2. Columns 1–10: well numbers. K: control for cell growth.

**Table S1:** Drug-likeness and bioavailability properties of modeled compounds.

Parameters	CTS	TLA	Glu
X log P3	-2.24	-1.88	-3.50
MW (Dalton)	189.21	150.09	179.17
TPSA (Å <sup>2</sup> )	84.16	115.06	116.17
log S	0.40	0.61	1.32
Csp <sup>3</sup>	1.00	0.50	1.00
Number of rotatable bonds	0	3	1
Bioavailability Score	0.55	0.56	0.55
Lipinski violations	0	0	0

**Table S2:** Molecular docking results to identify the protein-glucosamine interaction.

Complex	Energy (kcal/mol)		Conventional Hydrogen Bond		Other Interactions
	E <sub>vdw</sub>	E <sub>ele</sub>	Donor#H...Acceptor	Dist. (Å)	
1EQC-CTS	-38.82	-4.62	(E21)H...OH-C3	2.59	E186, E286, W357
			(Y23)H...OH-C4	2.11	
			(N185)H...OH-C2	2.04	
			2C-OH...O(E286)	2.89	
1EQC-Glu	-28.67	-5.50	(Y23)H...OH-C1	1.87	E286 and L298
			(Y23)H...OH-C3	2.51	
			(N140)H...C1-O-C6	2.47	
			1C-OH...O(E21)	1.85	
			6C-OH...O(L298)	2.15	
			2C-NHa...O(E186)	2.98	
			2C-NHa...O(E286)	2.51	
1K2Y-TLA	-13.77	-57.51	(H109)ND2...OH-C1	3.11	Zn464
			(K118)N...O=C1	2.94	
			(K118)N...OH-C2	3.04	
			(K118)N...OH-C3	3.17	
			(R247)NE...OH-C1	2.84	
			(R247)NH2...OH-C2	2.75	
1K2Y-Glu	-15.99	-9.25	1C-OH...N(H308)	2.44	R15, D18, D246, H329
			6C-OH...O(D18)	2.86	

**Table S3:** The radial distribution function (RDF) analysis: The  $n(r)$  up to the first minimum for the oxygen and nitrogen atoms of Glu.

Atoms	1EQC-Glu		1K2Y-Glu	
	Distance (nm)	$n(r)$	Distance (nm)	$n(r)$
1C-O-C6	0.33	0.57	0.38	1.77
1C-OH	0.38	1.63	0.36	2.27
3C-OH	0.37	1.00	0.31	1.14
4C-OH	0.43	2.50	0.38	2.23
6C-OH	-	-	0.32	1.37
2C-NH <sub>2</sub>	0.41	2.81	0.39	2.89

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