Table 1: OPLS Statistics from model correlating biofilm and planktonic growth of *P. spp.* in the presence of aluminium with computationally modeled chemical speciation concentrations of all predicted species in high phosphate, low phosphate and MOPS buffered media.

	R^2X	R^2Y	Q^2	CV-ANOVA (p)
Model (Total)	0.976	0.825	0.788	4.49×10^{-9}
Predicted (1)	0.363	0.793	0.745	
Predicted (2)	0.390	0.0313	0.0431	
Orthogonal	0.223	0.000962		
Orthogonal (1)	0.101	0.0000579		
Orthogonal (2)	0.123	0.000904		

Table 2: OPLS Statistics from model correlating biofilm and planktonic growth of *P. spp.* in the presence of aluminium with computationally modeled chemical speciation concentrations of only aluminium predicted species in high phosphate, low phosphate and MOPS buffered media.

	R^2X	R^2Y	Q^2	CV-ANOVA (p)
Model (Total)	0.999	0.771	0.746	1.11×10^{-10}
Predicted (1)	0.364	0.745	0.746	
Orthogonal	0.636	0.0259		
Orthogonal (1)	0.62	0.000804		
Orthogonal (2)	0.0152	0.0251		

Table 3: OPLS Statistics from model correlating biofilm and planktonic growth of *P. spp.* in the presence of copper with computationally modeled chemical speciation concentrations of all predicted species in high phosphate, low phosphate and MOPS buffered media.

	R^2X	R^2Y	Q^2	CV-ANOVA (p)
Model (Total)	0.976	0.791	0.738	7.51×10^{-13}
Predicted (1)	0.517	0.604	0.366	
Predicted (2)	0.203	0.187	0.372	
Orthogonal	0.256	0.0000381		
Orthogonal (1)	0.256	0.0000381		

Table 4: OPLS Statistics from model correlating biofilm and planktonic growth of *P. spp.* in the presence of copper with computationally modeled chemical speciation concentrations of only copper predicted species in high phosphate, low phosphate and MOPS buffered media.

	R^2X	R^2Y	Q^2	CV-ANOVA (p)
Model	1	0.228	0.18	0.944
1	0.631	0.218	0.179	
2	0.059	0.00972	0.00133	
Orthogonal	0.31	0		
1	0.31	0		

Table 5: OPLS Statistics from model correlating biofilm and planktonic growth of *P. spp.* in the presence of aluminium with computationally modeled chemical speciation concentrations of all predicted species in high phosphate buffered media with succinate, butyrate and benzoic acid as carbon sources.

	R^2X	R^2Y	Q^2	CV-ANOVA (p)
Model (Total)	0.997	0.88	0.839	8.01×10^{-8}
Predicted (1)	0.426	0.863	0.0819	
Predicted (2)	0.233	0.0121	0.00635	
Predicted (3)	0.0931	0.00442	0.0132	
Orthogonal	0.246	0		
Orthogonal (1)	0.157	0		
Orthogonal (2)	0.0893	0		

Table 6: OPLS Statistics from model correlating biofilm and planktonic growth of *P. spp.* in the presence of aluminium with computationally modeled chemical speciation concentrations of only aluminium predicted species in high phosphate buffered media with succinate, butyrate and benzoic acid as carbon sources.

	R^2X	R^2Y	Q^2	CV-ANOVA (p)
Model (Total)	0.996	0.691	0.646	1.73×10^{-7}
Predicted (1)	0.26	0.691	0.646	
Orthogonal	0.736	0.000697		
Orthogonal (1)	0.736	0.000697		

Table 7: OPLS Statistics from model correlating biofilm and planktonic growth of *P. spp.* in the presence of copper with computationally modeled chemical speciation concentrations of all predicted species in high phosphate buffered media with succinate, butyrate and benzoic acid as carbon sources.

	R2X	R2Y	Q2	CV-ANOVA (p)
Model (Total)	0.998	0.774	0.71	1.01×10^{-4}
Predicted (1)	0.408	0.562	0.484	
Predicted (2)	0.119	0.209	0.226	
Orthogonal	0.472	0.00362		
Orthogonal (1)	0.318	0.000283		
Orthogonal (2)	0.0977	0.00175		
Orthogonal (3)	0.0564	0.00158		

Table 8: OPLS Statistics from model correlating biofilm and planktonic growth of *P. spp.* in the presence of copper with computationally modeled chemical speciation concentrations of only copper predicted species in high phosphate buffered media with succinate, butyrate and benzoic acid as carbon sources.

	R2X	R2Y	Q2	CV-ANOVA (p)
Model (Total)	1	0.679	0.665	4.57×10^{-9}
Predicted (1)	0.999	0.492	0.356	
Predicted (2)	0.000181	0.187	0.309	