

Table S1. Thermodynamic parameters derived for boscalid-SiO₂ (E551) interaction in water using multiple sites model.

Parameters	Value
K _{d1} (M)	1.299E-9
K _{d2} (M)	1.012E-6
n1	0.492
n2	2.921
ΔH ₁ (kJ/mol)	-36.38
ΔH ₂ (kJ/mol)	-67.75
ΔS ₁ (J/mol·K)	4.819E1
ΔS ₂ (J/mol·K)	-1.125E2

Table S2 Simulated digestion stock and working solutions

Solution	Chemical	Mass/Volume	MW	Molarity	N ions	Osmolarity (Osm)
5 mM Phosphate buffer pH 7.0						
	Potassium Phosphate	0.6 g	136.09	.005	2	.010
	titrants (HCl, NaOH)					negl.
						Total: 0.010
Artificial Saliva Stock Solution (ASSS)						
	Sodium chloride	1.594 g	58.44	.0273	2	.0546
	Ammonium nitrate	0.328 g	80.05	.0041	2	.0082
	Potassium phosphate	0.636 g	136.09	.0047	2	.0094
	Potassium chloride	0.202 g	74.55	.0027	2	.0054
	Potassium citrate (monohydrate)	0.308 g	324.41	.0009	2	.0018
	Uric acid sodium salt	0.021 g	190.09	.0001	2	.0002
	Urea	0.198 g	60.06	.0033	1	.0066
	Lactic acid sodium salt (Sodium DL-lactate)	0.146 g	112.06	.0013	2	.0026
						Total: 0.0888
Artificial Saliva Work Solution (ASWS)						
	ASSS	20 ml				0.0888
	Porcine gastric mucin type II	0.6g			1	negl.
						Total: 0.0888
Simulated Gastric Fluid Stock Solution (SGFSS)						
	Sodium chloride	2 g	58.44	0.342	2	0.684

