

Run	Training results	15 PCs	20 PCs	Test samples	Test results	15 PCs	20 PCs	
1	α	0.0009	0.0057	10 ² CFU/ml	β	0.1308	-	
	Samples	80	80		Samples	20	-	
	Extremes	0	0		Externals	18	-	
	Outliers	0	0		β	0.1364	-	
	Notes			The extreme plot shows outliers.	10 ⁴ CFU/ml	Samples	20	-
					Externals	18	-	
					10 ⁶ CFU/ml	β	0.010	-
					Samples	20	-	
Externals	20	-						
2	α	0.015	0.024	10 ² CFU/ml	β	0.0691	5.2699e-05	
	Samples	80	80		Samples	20	20	
	Extremes	0	0		Externals	20	20	
	Outliers	0	0		β	0.003	7.6536e-05	
	Notes			The extreme plot shows a couple of outliers.	10 ⁴ CFU/ml	Samples	20	20
					Externals	20	20	
					10 ⁶ CFU/ml	β	0.0002	3.951e-07
					Samples	20	20	
Externals	20	20						
3	α	0.0063	0.0296	10 ² CFU/ml	β	0.0214	0.0008	
	Samples	80	80		Samples	20	20	
	Extremes	0	0		Externals	20	20	
	Outliers	0	0		β	0.0005	1.1640e-05	
	Notes				10 ⁴ CFU/ml	Samples	20	20
					Externals	20	20	
					10 ⁶ CFU/ml	β	0.0007	7.5937e-06
					Samples	20	20	
Externals	20	20						
4	α	0.0153	0.0221	10 ² CFU/ml	β	0.0872	0.0061	
	Samples	80	80		Samples	20	20	
	Extremes	0	0		Externals	20	20	
	Outliers	0	0		β	0.0505	0.0032	
	Notes				10 ⁴ CFU/ml	Samples	20	20
					Externals	20	20	
					10 ⁶ CFU/ml	β	0.001	9.2492e-07
					Samples	20	20	
Externals	20	20						
5	α	0.0051	0.0166	10 ² CFU/ml	β	0.0117	2.1159e-05	
	Samples	80	80		Samples	20	20	
	Extremes	0	0		Externals	19	20	
	Outliers	0	0		β	0.0056	5.9069e-05	
	Notes				10 ⁴ CFU/ml	Samples	20	20
					Externals	20	20	
					10 ⁶ CFU/ml	β	0.9084	0
					Samples	20	20	
Externals	18	20						
6	α	0.0232	0.0270	10 ² CFU/ml	β	0.06199	-	
	Samples	80	80		Samples	20	-	
	Extremes	0	0		Externals	19	-	
	Outliers	0	0		β	8.4298e-05	-	
	Notes			The extreme plot shows outliers.	10 ⁴ CFU/ml	Samples	20	-
					Externals	20	-	
					10 ⁶ CFU/ml	β	2.5971e-05	-
					Samples	20	-	
Externals	20	-						
7	α	0.0048	0.0045	10 ² CFU/ml	β	0.1283	0.0119	
	Samples	80	80		Samples	20	20	
	Extremes	0	0		Externals	20	20	
	Outliers	0	0		β	NaN	NaN	
	Notes			The extreme plot shows a couple of outliers.	10 ⁴ CFU/ml	Samples	20	20
					Externals	20	20	
					10 ⁶ CFU/ml	β	0.0021	1.2783e-05
					Samples	20	20	
Externals	20	20						
8	α	0.0018	0.0155	10 ² CFU/ml	β	0.1117	0.0005	
	Samples	20	20		Samples	20	20	
	Extremes	0	0		Externals	19	20	
	Outliers	0	0		β	0.2548	0.0015	
	Notes				10 ⁴ CFU/ml	Samples	20	20
					Externals	19	20	
					10 ⁶ CFU/ml	β	0.0013	2.7799e-06
					Samples	20	20	

					Samples	20	20	
					Externals	20	20	
9	α	0.0078	0.0018	10 ² CFU/ml	β	0.0777	0.0051	
	Samples	80	80		Samples	20	20	
	Extremes	0	0		Externals	20	20	
	Outliers	0	0	10 ⁴ CFU/ml	β	0.0594	0.0015	
	Notes				<i>The extreme plot shows a couple of outliers.</i>	Samples	20	20
				Externals		20	20	
				β		0.0058	0.0001	
				Samples		20	20	
				10 ⁶ CFU/ml	Externals	20	20	
10	α	0.0185	0.0104	10 ² CFU/ml	β	0.0279	0.0029	
	Samples	80	80		Samples	20	20	
	Extremes	0	0		Externals	20	20	
	Outliers	0	0	10 ⁴ CFU/ml	β	0	0	
	Notes				Samples	20	20	
				Externals	20	20		
				β	5.4578	0		
				Samples	20	20		
					10 ⁶ CFU/ml	Externals	20	20

Table S1. The DD-SIMCA model results. The yellow boxes represent the simulations in which the model did not identify as extraneous respect to the current model all the test samples.