

Supplementary Table

method	R ² (squared r-coefficient)	RMSE (°C)	RMSD (°C)
CoDa-PLSR			
<i>15 taxa 2 groups annual</i>	0.9351 (0.9718)	1.3349	
<i>15 taxa 2 groups robust annual</i>	0.9060 (0.9591)	1.7571	
<i>15 taxa 2 groups summer</i>	0.8796 (0.9533)	1.6567	2.3007
<i>15 taxa 2 groups winter</i>	0.9206 (0.9609)	1.5964	
<i>19 taxa 2 groups annual</i>	0.9315 (0.9702)	1.3716	
<i>19 taxa 2 groups summer</i>	0.8741 (0.9512)	1.6945	2.3414
<i>19 taxa 2 groups winter</i>	0.9186 (0.9599)	1.6158	
<i>15 taxa annual</i>	0.9367	1.9985	
<i>15 taxa summer</i>	0.917	2.2054	3.1871
<i>15 taxa winter</i>	0.9188	2.3008	
<i>19 taxa annual</i>	0.9326	2.0625	
CoDa-PCR			
<i>15 taxa 2 groups annual</i>	0.9276 (0.9686)	1.5651	
<i>15 taxa 2 groups summer</i>	0.8678 (0.9487)	1.7364	2.3927
<i>15 taxa 2 groups winter</i>	0.8781 (0.9645)	1.6462	
<i>15 taxa 2 groups robust</i>	0.9262 (0.9685)	1.4103	
<i>15 taxa annual</i>	0.9210	2.2323	
<i>15 taxa summer</i>	0.8933	2.5071	3.4350
<i>15 taxa winter</i>	0.9149	2.3621	
Coda-MAT			
<i>CoDa-MAT annual</i>	0.9857	0.9484	

Cross-validation results for ilr/clr-PLSR ilr/clr-PCR, obtained under different conditions.