

Table S1 The partition of sample set

Statistical parameter	Capsaicin (g/kg)			Dihydrocapsaicin (g/kg)			Pungency degree (SHU)		
	Calibration set	validation set	Prediction set	Calibration set	validation set	Prediction set	Calibration set	validation set	Prediction set
Max	2.610	2.160	1.810	1.940	1.000	1.870	61191.00	53794.50	60919.50
Min	0.480	0.780	0.760	0.150	0.320	0.450	11916.00	18922.50	31224.00
Mean	1.556	1.573	1.068	0.650	0.606	1.384	37573.01	37316.00	42653.78
Standard deviation	0.480	0.385	0.213	0.255	0.179	0.290	10754.45	9201.20	7132.86

Table S2 Results of the full spectra by different pretreatment methods

Parts of pepper	Pretreatment	LV	Rcv	RMSEcv	RPDev	Rv	RMSEpv	RPDv
Near stalk-end location	Raw	8	0.496	0.438	1.095	0.553	0.329	1.170
	De Bias	10	0.540	0.422	1.138	0.553	0.335	1.148
	DT	11	0.568	0.412	1.166	0.577	0.324	1.186
	SNV	8	0.544	0.422	1.138	0.557	0.333	1.155
	Min Max	8	0.514	0.433	1.108	0.552	0.329	1.171
	MSC	8	0.545	0.422	1.138	0.557	0.333	1.155
	1st	8	0.552	0.410	1.170	0.542	0.326	1.180
	2nd	8	0.577	0.401	1.196	0.552	0.330	1.167
	1st-DT	8	0.550	0.410	1.170	0.536	0.327	1.177
	1st-SNV	8	0.516	0.429	1.118	0.497	0.339	1.136
	1st-MSC	8	0.527	0.424	1.131	0.498	0.339	1.135
	CWT	8	0.518	0.427	1.125	0.541	0.327	1.178
	CWT-MSC	8	0.513	0.431	1.114	0.523	0.332	1.160
	CWT-SNV	8	0.503	0.435	1.103	0.518	0.333	1.156
Capsaicin	Raw	10	0.586	0.376	1.198	0.346	0.388	1.051
	De Bias	8	0.553	0.386	1.167	0.306	0.395	1.034
	DT	8	0.572	0.377	1.193	0.231	0.409	0.999
	SNV	8	0.558	0.384	1.171	0.296	0.402	1.016
	Min Max	8	0.534	0.392	1.149	0.293	0.398	1.025
	MSC	8	0.556	0.385	1.171	0.293	0.402	1.017
	1st	8	0.590	0.371	1.214	0.408	0.375	1.088
	2nd	8	0.561	0.382	1.177	0.367	0.389	1.051
	1st-DT	8	0.593	0.370	1.217	0.401	0.378	1.082
	1st-SNV	8	0.573	0.378	1.192	0.277	0.413	0.989
	1st-MSC	8	0.574	0.377	1.195	0.282	0.407	1.004
	CWT	8	0.573	0.377	1.193	0.339	0.391	1.045
	CWT-MSC	8	0.562	0.381	1.181	0.288	0.401	1.018
	CWT-SNV	8	0.568	0.379	1.187	0.283	0.405	1.007
	Raw	9	0.532	0.408	1.160	0.381	0.316	1.042
	De Bias	8	0.523	0.411	1.151	0.384	0.316	1.044
	DT	8	0.534	0.406	1.165	0.320	0.329	1.001
	SNV	8	0.546	0.408	1.160	0.378	0.319	1.033
	Min Max	8	0.542	0.409	1.158	0.343	0.319	1.032
	MSC	8	0.545	0.408	1.159	0.377	0.319	1.033
Near navel-end location	1st	8	0.508	0.415	1.140	0.400	0.314	1.051
	2nd	8	0.491	0.427	1.108	0.315	0.352	0.937
	1st-DT	8	0.501	0.418	1.133	0.393	0.314	1.049
	1st-SNV	8	0.488	0.429	1.105	0.398	0.330	0.998
	1st-MSC	8	0.496	0.424	1.118	0.384	0.335	0.984
	CWT	8	0.517	0.412	1.149	0.364	0.326	1.010
	CWT-MSC	8	0.510	0.420	1.129	0.349	0.347	0.949
	CWT-SNV	8	0.504	0.423	1.119	0.371	0.342	0.963

Table S2 (Continued)

	Parts of pepper	Pretreatment	LV	Rcv	RMSEcv	RPDcv	Rv	RMSEPv	RPDv
Capsaicin	Average spectra	Raw	8	0.607	0.360	1.245	0.444	0.386	1.115
		De Bias	10	0.608	0.360	1.246	0.320	0.432	0.996
		DT	8	0.583	0.369	1.216	0.365	0.413	1.043
		SNV	8	0.602	0.361	1.241	0.350	0.427	1.008
		Min Max	8	0.594	0.364	1.232	0.405	0.406	1.062
		MSC	8	0.595	0.364	1.232	0.356	0.424	1.015
		1st	8	0.581	0.369	1.215	0.329	0.424	1.017
		2nd	8	0.554	0.382	1.175	0.279	0.435	0.990
		1st-DT	8	0.581	0.369	1.216	0.329	0.422	1.020
		1st-SNV	8	0.606	0.360	1.244	0.218	0.456	0.946
		1st-MSC	8	0.570	0.375	1.196	0.232	0.449	0.960
		CWT	8	0.589	0.366	1.226	0.300	0.430	1.001
		CWT-MSC	8	0.575	0.376	1.192	0.268	0.433	0.995
		CWT-SNV	8	0.614	0.360	1.247	0.234	0.455	0.948
Dihydrocapsaicin	Near stalk- end location	Raw	8	0.554	0.192	1.180	0.450	0.161	1.114
		De Bias	8	0.525	0.196	1.154	0.501	0.154	1.163
		DT	8	0.528	0.195	1.160	0.458	0.160	1.118
		SNV	8	0.504	0.202	1.121	0.530	0.151	1.184
		Min Max	8	0.504	0.199	1.136	0.533	0.150	1.193
		MSC	8	0.503	0.202	1.119	0.528	0.152	1.181
		1st	8	0.495	0.202	1.118	0.377	0.169	1.061
		2nd	8	0.488	0.205	1.105	0.487	0.159	1.127
		1st-DT	8	0.497	0.202	1.121	0.381	0.169	1.059
		1st-SNV	8	0.513	0.199	1.139	0.374	0.168	1.067
		1st-MSC	8	0.490	0.204	1.108	0.354	0.171	1.048
		CWT	8	0.502	0.201	1.125	0.442	0.163	1.100
		CWT-MSC	8	0.512	0.199	1.139	0.443	0.163	1.102
		CWT-SNV	8	0.509	0.199	1.135	0.462	0.159	1.127
	Equatorial location	Raw	8	0.592	0.212	1.166	0.201	0.201	0.985
		De Bias	8	0.555	0.210	1.172	0.257	0.196	1.010
		DT	8	0.591	0.202	1.219	0.179	0.204	0.973
		SNV	8	0.626	0.198	1.246	0.217	0.206	0.963
		Min Max	8	0.588	0.203	1.215	0.174	0.200	0.993
		MSC	8	0.617	0.200	1.233	0.210	0.205	0.968
		1st	8	0.637	0.194	1.275	0.251	0.199	0.998
		2nd	8	0.575	0.209	1.180	0.299	0.194	1.022
		1st-DT	8	0.636	0.193	1.275	0.244	0.200	0.993
		1st-SNV	8	0.645	0.191	1.293	0.280	0.202	0.979
		1st-MSC	8	0.626	0.195	1.265	0.259	0.199	0.997
		CWT	8	0.646	0.191	1.294	0.233	0.200	0.989
		CWT-MSC	8	0.624	0.196	1.258	0.271	0.196	1.009
		CWT-SNV	8	0.652	0.189	1.304	0.274	0.201	0.984

Table S2 (Continued)

Parts of pepper		Pretreatment	LV	Rcv	RMSEcv	RPDcv	Rv	RMSEPv	RPDv
Dihydrocapsaicin	Near navel- end location	Raw	8	0.399	0.221	1.026	0.034	0.178	0.895
		De Bias	8	0.400	0.218	1.039	0.084	0.173	0.918
		DT	8	0.394	0.218	1.038	-0.072	0.189	0.842
		SNV	8	0.405	0.218	1.040	0.010	0.189	0.842
		Min Max	8	0.412	0.217	1.044	-0.067	0.188	0.845
		MSC	8	0.388	0.220	1.028	0.000	0.191	0.834
		1st	12	0.458	0.217	1.044	-0.232	0.212	0.748
		2nd	8	0.323	0.243	0.934	0.013	0.187	0.848
		1st-DT	12	0.464	0.215	1.052	-0.213	0.214	0.742
		1st-SNV	8	0.492	0.204	1.109	0.043	0.188	0.847
		1st-MSC	8	0.446	0.213	1.065	-0.043	0.200	0.795
		CWT	12	0.438	0.219	1.036	-0.260	0.221	0.720
		CWT-MSC	8	0.415	0.218	1.041	-0.073	0.199	0.800
		CWT-SNV	8	0.442	0.212	1.070	0.003	0.192	0.829
	Average spectra	Raw	8	0.554	0.204	1.156	0.153	0.162	0.902
		De Bias	8	0.540	0.203	1.166	0.144	0.172	0.850
		DT	8	0.541	0.203	1.162	0.153	0.169	0.866
		SNV	8	0.532	0.207	1.143	0.117	0.180	0.811
		Min Max	8	0.513	0.211	1.120	0.102	0.180	0.811
		MSC	8	0.516	0.210	1.127	0.119	0.179	0.816
		1st	8	0.545	0.203	1.160	0.096	0.171	0.854
		2nd	8	0.490	0.215	1.096	0.132	0.170	0.859
		1st-DT	8	0.544	0.203	1.161	0.095	0.171	0.854
		1st-SNV	8	0.586	0.195	1.213	0.159	0.165	0.884
		1st-MSC	8	0.550	0.202	1.169	0.154	0.165	0.884
		CWT	8	0.548	0.203	1.162	0.084	0.171	0.856
		CWT-MSC	8	0.532	0.207	1.142	0.193	0.167	0.873
		CWT-SNV	8	0.596	0.193	1.222	0.182	0.170	0.857
Pungency degree	Near stalk- end location	Raw	11	0.520	63.381	1.131	0.537	54.555	1.124
		De Bias	8	0.452	66.247	1.082	0.524	53.412	1.148
		DT	8	0.478	64.866	1.105	0.521	54.993	1.115
		SNV	8	0.476	65.104	1.101	0.530	53.770	1.141
		Min Max	8	0.443	66.714	1.075	0.540	52.235	1.174
		MSC	8	0.477	65.025	1.103	0.530	53.768	1.141
		1st	8	0.481	64.795	1.107	0.514	53.193	1.153
		2nd	8	0.478	65.196	1.100	0.544	52.449	1.170
		1st-DT	8	0.482	64.523	1.111	0.513	53.070	1.156
		1st-SNV	8	0.412	69.427	1.033	0.461	55.285	1.110
		1st-MSC	8	0.439	67.770	1.058	0.461	55.244	1.110
		CWT	8	0.460	66.405	1.080	0.518	53.272	1.151
		CWT-MSC	8	0.442	67.436	1.063	0.519	52.703	1.164
		CWT-SNV	8	0.423	68.586	1.045	0.520	52.654	1.165

Table S2 (Continued)

Parts of	Pretreatment	LV	Rcv	RMSEcv	RPDcv	Rv	RMSEPv	RPDv
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pepper									
Pungency degree	Equatorial location	Raw	8	0.456	61.314	1.076	0.322	62.293	1.044
		De Bias	8	0.362	66.966	0.985	0.307	62.638	1.038
		DT	8	0.355	66.151	0.998	0.376	60.161	1.081
		SNV	8	0.386	64.988	1.015	0.215	66.854	0.973
		Min Max	8	0.340	66.899	0.986	0.390	59.801	1.088
		MSC	8	0.381	65.024	1.015	0.216	66.386	0.980
		1st	8	0.425	63.474	1.040	0.425	58.802	1.106
		2nd	8	0.360	66.709	0.989	0.446	58.011	1.121
		1st-DT	8	0.431	62.979	1.048	0.426	58.826	1.106
		1st-SNV	8	0.472	59.964	1.100	0.318	64.282	1.012
		1st-MSC	8	0.451	60.987	1.082	0.311	63.395	1.026
		CWT	8	0.441	62.189	1.061	0.371	60.894	1.068
		CWT-MSC	8	0.435	62.197	1.061	0.362	60.856	1.069
		CWT-SNV	8	0.459	61.090	1.080	0.362	61.664	1.055
		Raw	8	0.361	69.237	1.010	0.348	49.991	1.034
		De Bias	8	0.365	66.895	1.046	0.326	50.673	1.020
	DT	8	0.335	68.608	1.020	0.180	56.490	0.915	
	SNV	8	0.403	66.954	1.045	0.236	55.719	0.927	
	Min Max	8	0.390	66.599	1.050	0.280	53.254	0.970	
	MSC	8	0.395	67.300	1.039	0.229	56.082	0.921	
	1st	8	0.340	68.811	1.017	0.272	53.741	0.962	
	2nd	8	0.276	73.867	0.947	0.228	57.240	0.903	
	1st-DT	8	0.328	69.262	1.010	0.257	54.021	0.957	
	1st-SNV	8	0.328	69.819	1.002	0.274	56.409	0.916	
	1st-MSC	8	0.329	69.771	1.003	0.235	58.167	0.888	
	CWT	8	0.297	70.873	0.987	0.254	54.821	0.943	
	CWT-MSC	8	0.330	69.927	1.000	0.224	58.609	0.882	
	CWT-SNV	8	0.333	69.822	1.002	0.264	57.206	0.903	
	Average spectra	Raw	8	0.481	59.820	1.122	0.393	59.889	1.056
		De Bias	8	0.415	62.825	1.069	0.330	63.458	0.997
		DT	8	0.408	63.032	1.065	0.297	64.290	0.984
		SNV	8	0.515	58.402	1.150	0.290	66.712	0.948
Min Max		8	0.422	62.358	1.077	0.335	64.047	0.988	
MSC		8	0.493	59.323	1.132	0.297	66.143	0.956	
1st		8	0.378	64.737	1.037	0.282	65.083	0.972	
2nd		8	0.376	66.492	1.010	0.229	66.737	0.948	
1st-DT		8	0.383	64.352	1.043	0.281	64.844	0.976	
1st-SNV		8	0.465	60.765	1.105	0.206	68.603	0.922	
1st-MSC		8	0.416	62.950	1.067	0.184	69.187	0.914	
CWT		8	0.389	63.913	1.050	0.258	65.723	0.963	
CWT-MSC		8	0.389	64.026	1.049	0.219	66.189	0.956	
CWT-SNV		8	0.459	61.306	1.095	0.211	68.911	0.918	

Table S3 Results of prediction set with the full spectra and best pretreatment method

Parts of pepper		Pretreatment	Rp	RMSEpp	RPDp
Capsaicin	Near stalk-end location	DT	0.326	0.440	0.483

Dihydrocapsaicin	Equatorial location	1st	0.003	0.394	0.540
	Near navel-end location	1st	0.159	0.462	0.470
	Average spectra	Raw	0.467	0.395	0.550
	Near stalk-end location	Min Max	0.261	0.504	0.380
	Equatorial location	2nd	0.162	0.529	0.505
	Near navel-end location	De Bias	-0.379	0.659	0.394
	Average spectra	CWT-MSC	0.222	0.513	0.473
	Near stalk-end location	2nd	0.336	101.561	0.468
	Equatorial location	2nd	0.260	63.232	0.762
	Near navel-end location	Raw	0.121	67.556	0.708
Pungency degree	Average spectra	Raw	0.478	45.757	1.011

Table S4 Results of the spectra in the range of 969 to 1619 nm by different pretreatment methods

Parts of pepper	Pretreatment	LV	Rcv	RMSEcv	RPDcv	Rv	RMSEpv	RPDv
Near navel-end location	Raw	11	0.567	0.386	1.182	0.627	0.341	1.277
	De Bias	10	0.588	0.375	1.216	0.615	0.344	1.264
	DT	10	0.514	0.404	1.129	0.699	0.316	1.375
	SNV	11	0.613	0.371	1.230	0.577	0.368	1.183
	Min Max	9	0.567	0.383	1.192	0.644	0.338	1.288
	MSC	9	0.620	0.363	1.258	0.578	0.363	1.198
	1st	12	0.614	0.372	1.225	0.684	0.315	1.381
	2nd	8	0.487	0.418	1.092	0.693	0.317	1.372
	1st-DT	8	0.529	0.394	1.158	0.694	0.322	1.352
	1st-SNV	8	0.513	0.405	1.125	0.670	0.338	1.287
	1st-MSC	8	0.528	0.402	1.136	0.730	0.302	1.440
	CWT	10	0.602	0.373	1.222	0.672	0.324	1.344
	CWT-MSC	8	0.530	0.400	1.140	0.726	0.305	1.426
	CWT-SNV	8	0.519	0.402	1.133	0.666	0.340	1.278
	Raw	11	0.586	0.401	1.205	0.437	0.302	1.064
Capsaicin	De Bias	10	0.595	0.397	1.219	0.459	0.292	1.099
	DT	9	0.589	0.397	1.219	0.409	0.305	1.053
	SNV	8	0.617	0.383	1.262	0.500	0.279	1.152
	Min Max	10	0.626	0.384	1.260	0.435	0.304	1.058
	MSC	8	0.604	0.388	1.246	0.500	0.280	1.147
	1st	9	0.630	0.380	1.271	0.547	0.288	1.118
	2nd	8	0.441	0.466	1.038	0.431	0.304	1.056
	1st-DT	9	0.607	0.389	1.242	0.416	0.313	1.025
	1st-SNV	8	0.601	0.394	1.226	0.419	0.308	1.043
	1st-MSC	8	0.612	0.387	1.251	0.417	0.309	1.041
	CWT	9	0.635	0.378	1.279	0.540	0.287	1.119
	CWT-MSC	8	0.620	0.383	1.264	0.418	0.308	1.044
	CWT-SNV	8	0.599	0.395	1.225	0.422	0.307	1.048
	Raw	9	0.496	0.411	1.125	0.387	0.354	1.073
	De Bias	11	0.510	0.408	1.132	0.481	0.353	1.076
Near navel-end location	DT	8	0.420	0.435	1.062	0.530	0.320	1.186
	SNV	9	0.530	0.400	1.155	0.524	0.324	1.172
	Min Max	9	0.539	0.398	1.161	0.468	0.345	1.100
	MSC	9	0.513	0.406	1.140	0.455	0.344	1.103
	1st	8	0.448	0.425	1.088	0.466	0.334	1.137
	2nd	8	0.365	0.464	0.996	0.501	0.340	1.115
	1st-DT	8	0.332	0.463	0.998	0.569	0.309	1.230
	1st-SNV	8	0.399	0.444	1.042	0.557	0.312	1.215
	1st-MSC	8	0.444	0.427	1.083	0.595	0.301	1.260
	CWT	8	0.446	0.426	1.087	0.456	0.336	1.129
	CWT-MSC	8	0.436	0.429	1.078	0.601	0.301	1.262
	CWT-SNV	8	0.382	0.448	1.033	0.562	0.312	1.217

Table S4 (Continued)

	Parts of pepper	Pretreatment	LV	Rcv	RMSEcv	RPDcv	Rv	RMSEPv	RPDv
Capsaicin	Average spectra	Raw	12	0.599	0.369	1.234	0.393	0.398	1.067
		De Bias	12	0.622	0.361	1.261	0.332	0.412	1.030
		DT	12	0.614	0.366	1.245	0.241	0.422	1.005
		SNV	12	0.641	0.355	1.283	0.417	0.391	1.087
		Min Max	12	0.652	0.348	1.309	0.369	0.405	1.048
		MSC	12	0.650	0.350	1.302	0.392	0.398	1.068
		1st	12	0.644	0.353	1.291	0.526	0.361	1.177
		2nd	12	0.578	0.382	1.191	0.402	0.412	1.031
		1st-DT	12	0.604	0.372	1.223	0.473	0.378	1.123
		1st-SNV	12	0.620	0.367	1.240	0.431	0.387	1.096
		1st-MSC	11	0.616	0.367	1.242	0.366	0.404	1.052
		CWT	12	0.645	0.352	1.293	0.525	0.362	1.174
		CWT-MSC	11	0.620	0.365	1.249	0.399	0.397	1.070
		CWT-SNV	12	0.618	0.369	1.235	0.469	0.378	1.125
Dihydrocapsaicin	Near stalk- end location	Raw	11	0.642	0.182	1.286	0.516	0.165	1.182
		De Bias	12	0.644	0.183	1.284	0.422	0.175	1.114
		DT	9	0.636	0.183	1.279	0.536	0.163	1.198
		SNV	11	0.637	0.184	1.273	0.446	0.173	1.129
		Min Max	11	0.627	0.186	1.260	0.437	0.173	1.126
		MSC	10	0.635	0.184	1.276	0.483	0.169	1.155
		1st	9	0.665	0.177	1.322	0.495	0.167	1.165
		2nd	8	0.621	0.188	1.244	0.554	0.163	1.198
		1st-DT	9	0.652	0.180	1.300	0.541	0.162	1.202
		1st-SNV	9	0.644	0.183	1.280	0.560	0.161	1.211
		1st-MSC	8	0.637	0.183	1.279	0.554	0.161	1.214
		CWT	9	0.662	0.178	1.319	0.481	0.169	1.154
		CWT-MSC	8	0.640	0.182	1.285	0.537	0.162	1.200
		CWT-SNV	8	0.635	0.183	1.279	0.561	0.161	1.213
	Equatorial location	Raw	8	0.715	0.190	1.424	0.329	0.154	1.045
		De Bias	11	0.689	0.198	1.363	0.516	0.140	1.152
		DT	11	0.704	0.194	1.396	0.511	0.141	1.144
		SNV	11	0.706	0.193	1.403	0.504	0.141	1.143
		Min Max	9	0.704	0.193	1.401	0.424	0.148	1.088
		MSC	10	0.710	0.191	1.413	0.481	0.142	1.133
		1st	11	0.667	0.205	1.321	0.495	0.141	1.138
		2nd	8	0.554	0.236	1.144	0.383	0.155	1.041
		1st-DT	10	0.674	0.201	1.341	0.444	0.146	1.105
		1st-SNV	9	0.711	0.191	1.414	0.479	0.143	1.124
		1st-MSC	9	0.703	0.193	1.400	0.457	0.144	1.113
		CWT	11	0.668	0.204	1.322	0.483	0.143	1.127
		CWT-MSC	9	0.703	0.193	1.400	0.460	0.144	1.117
		CWT-SNV	9	0.715	0.190	1.424	0.476	0.143	1.127

Table S4 (Continued)

	Parts of pepper	Pretreatment	LV	Rcv	RMSEcv	RPDcv	Rv	RMSEPv	RPDv
Dihydrocapsaicin	Near navel- end location	Raw	8	0.435	0.267	1.286	0.352	0.170	1.182
		De Bias	8	0.545	0.207	1.284	0.423	0.176	1.114
		DT	8	0.444	0.225	1.279	0.403	0.164	1.198
		SNV	8	0.527	0.212	1.273	0.439	0.175	1.129
		Min Max	8	0.524	0.210	1.260	0.459	0.167	1.126
		MSC	8	0.544	0.207	1.276	0.431	0.178	1.155
		1st	9	0.539	0.208	1.322	0.373	0.189	1.165
		2nd	8	0.410	0.234	1.244	0.202	0.185	1.198
		1st-DT	9	0.480	0.218	1.300	0.380	0.174	1.202
		1st-SNV	8	0.458	0.224	1.280	0.372	0.166	1.211
		1st-MSC	8	0.475	0.220	1.279	0.369	0.180	1.214
		CWT	9	0.543	0.207	1.319	0.366	0.191	1.154
		CWT-MSC	8	0.474	0.222	1.285	0.366	0.178	1.200
		CWT-SNV	8	0.458	0.223	1.279	0.373	0.164	1.213
	Average spectra	Raw	12	0.630	0.192	1.424	0.408	0.161	1.045
		De Bias	12	0.645	0.188	1.363	0.374	0.166	1.152
		DT	11	0.626	0.191	1.396	0.204	0.185	1.144
		SNV	11	0.659	0.184	1.403	0.439	0.159	1.143
		Min Max	12	0.634	0.191	1.401	0.339	0.172	1.088
		MSC	11	0.658	0.185	1.413	0.375	0.167	1.133
		1st	10	0.649	0.186	1.321	0.427	0.160	1.138
		2nd	8	0.542	0.210	1.144	0.144	0.177	1.041
		1st-DT	10	0.601	0.197	1.341	0.290	0.173	1.105
		1st-SNV	10	0.627	0.191	1.414	0.285	0.172	1.124
		1st-MSC	9	0.613	0.194	1.400	0.238	0.179	1.113
		CWT	10	0.649	0.186	1.322	0.458	0.156	1.127
		CWT-MSC	10	0.620	0.193	1.400	0.264	0.175	1.117
		CWT-SNV	10	0.631	0.191	1.424	0.318	0.168	1.127
Pungency degree	Near stalk- end location	Raw	12	0.515	58.632	1.132	0.619	54.386	1.273
		De Bias	10	0.524	57.763	1.149	0.658	52.183	1.326
		DT	8	0.395	62.576	1.060	0.691	50.807	1.362
		SNV	8	0.492	58.834	1.128	0.610	56.453	1.226
		Min Max	8	0.491	58.855	1.127	0.715	51.161	1.353
		MSC	9	0.527	57.694	1.150	0.649	53.204	1.301
		1st	10	0.541	57.221	1.160	0.691	50.676	1.366
		2nd	8	0.388	64.848	1.023	0.746	47.917	1.445
		1st-DT	8	0.455	60.345	1.099	0.723	48.612	1.424
		1st-SNV	8	0.440	61.578	1.077	0.706	50.607	1.368
		1st-MSC	8	0.455	60.792	1.091	0.728	48.893	1.416
		CWT	10	0.547	56.837	1.167	0.686	50.900	1.360
		CWT-MSC	8	0.471	60.006	1.106	0.723	49.196	1.407
		CWT-SNV	8	0.454	60.779	1.092	0.699	51.010	1.357

Table S4 (Continued)

	Parts of	Pretreatment	LV	Rcv	RMSEcv	RPDcv	Rv	RMSEPv	RPDv
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pepper									
Pungency degree	Equatorial location	Raw	8	0.512	63.493	1.139	0.451	46.601	1.112
		De Bias	11	0.514	64.302	1.125	0.533	45.401	1.141
		DT	8	0.434	68.574	1.055	0.431	46.804	1.107
		SNV	10	0.547	62.225	1.162	0.496	46.617	1.111
		Min Max	9	0.546	61.960	1.167	0.477	46.175	1.122
		MSC	9	0.547	61.511	1.176	0.509	45.786	1.132
		1st	9	0.508	63.930	1.131	0.521	44.194	1.172
		2nd	8	0.317	79.001	0.915	0.569	42.868	1.209
		1st-DT	9	0.507	63.988	1.130	0.470	46.197	1.122
		1st-SNV	9	0.544	62.136	1.164	0.471	48.107	1.077
		1st-MSC	8	0.543	61.804	1.170	0.471	47.458	1.092
		CWT	9	0.525	62.782	1.152	0.519	44.251	1.171
		CWT-MSC	8	0.554	61.178	1.182	0.474	47.285	1.096
		CWT-SNV	9	0.562	60.881	1.188	0.481	47.134	1.099
		Raw	9	0.409	65.118	1.050	0.492	52.168	1.125
	De Bias	10	0.457	61.886	1.105	0.483	55.442	1.058	
	DT	8	0.234	71.887	0.952	0.524	49.384	1.188	
	SNV	8	0.407	63.767	1.073	0.467	53.406	1.099	
	Min Max	10	0.487	61.100	1.119	0.531	51.279	1.144	
	MSC	9	0.462	61.683	1.109	0.540	50.715	1.157	
	1st	11	0.418	64.992	1.052	0.525	53.954	1.088	
	2nd	8	0.151	78.779	0.868	0.444	55.940	1.049	
	1st-DT	8	0.069	78.317	0.873	0.572	48.580	1.208	
	1st-SNV	8	0.343	66.539	1.028	0.554	49.459	1.186	
	1st-MSC	8	0.351	66.740	1.025	0.555	50.433	1.163	
	CWT	10	0.407	64.501	1.060	0.566	49.185	1.193	
	CWT-MSC	8	0.345	66.900	1.022	0.555	50.357	1.165	
	CWT-SNV	8	0.333	66.811	1.024	0.553	49.326	1.190	
	Average spectra	Raw	12	0.572	57.481	1.192	0.353	62.551	1.022
		De Bias	11	0.573	56.986	1.202	0.360	61.844	1.034
DT		8	0.428	64.358	1.064	0.240	64.122	0.997	
SNV		10	0.585	56.459	1.213	0.528	53.816	1.188	
Min Max		11	0.577	57.053	1.201	0.345	63.308	1.010	
MSC		11	0.579	56.736	1.207	0.347	63.191	1.012	
1st		10	0.558	58.093	1.179	0.449	58.480	1.093	
2nd		8	0.430	64.202	1.067	0.225	65.558	0.975	
1st-DT		8	0.468	61.948	1.106	0.338	60.761	1.052	
1st-SNV		8	0.512	60.413	1.134	0.346	60.285	1.061	
1st-MSC		8	0.500	61.241	1.119	0.231	66.558	0.961	
CWT		10	0.560	57.970	1.182	0.468	57.635	1.109	
CWT-MSC		8	0.503	61.062	1.122	0.259	65.387	0.978	
CWT-SNV		8	0.515	60.112	1.140	0.367	59.505	1.074	

Table S5 Results of prediction set with the spectra in the range of 969 to 1619 nm

Parts of pepper		Pretreatment	Rp	RMSEPp	RPDp
Capsaicin	Near stalk-end location	1st-MSC	0.528	0.316	0.528

Dihydrocapsaicin	Equatorial location	1st	0.365	0.342	0.528
	Near navel-end location	CWT-MSC	0.029	0.370	0.599
	Average spectra	1st	0.075	0.327	0.665
	Near stalk-end location	CWT-SNV	0.376	0.598	0.436
	Equatorial location	De Bias	0.084	0.627	0.418
	Near navel-end location	Min Max	-0.368	0.667	0.386
	Average spectra	CWT	0.081	0.698	0.428
	Near stalk-end location	2nd	0.230	88.789	0.570
	Equatorial location	2nd	0.039	98.088	0.451
	Near navel-end location	1st-DT	0.070	106.740	0.429
Pungency degree	Average spectra	SNV	0.087	96.410	0.493