Table S1. Selected wavenumber variables retained after CARS and their corresponding wavelengths.

Number	Selected Wavenumber (cm-1)	Corresponding Wavelength (nm)
1	11840	844.5945946
2	11814	846.4533604
3	11756	850.6294658
4	11754	850.7742045
5	11668	857.0449092
6	11476	871.3837574
7	11474	871.5356458
8	11472	871.6875872
9	11470	871.8395815
10	11334	882.3010411
11	11332	882.4567596
12	11320	883.3922261
13	11318	883.5483301
14	11316	883.7044892
15	11176	894.7745168
16	11106	900.4141905
17	11104	900.5763689
18	11054	904.6499005
19	11000	909.0909091
20	10960	912.4087591
21	10958	912.5752875
22	10956	912.7418766
23	10948	913.4088418
24	10946	913.5757354
25	10944	913.7426901
26	10942	913.9097057
27	10920	915.7509158
28	10918	915.9186664
29	10916	916.0864786
30	10908	916.7583425
31	10906	916.9264625
32	10904	917.0946442
33	10780	927.6437848
34	10778	927.8159213
35	10776	927.9881218
36	10734	931.6191541
37	10696	934.9289454
38	10694	935.1037965
39	10692	935.2787131
40	10690	935.453695
41	10664	937.7344336
42	10662	937.9103358

Table S1 (continued)

Number	Selected Wavenumber (cm-1)	Corresponding Wavelength (nm)
43	10648	939.1435011
44	10646	939.3199324
45	10644	939.4964299
46	10406	960.9840477
47	10404	961.1687812
48	10402	961.3535858
49	10376	963.7625289
50	10366	964.6922632
51	10364	964.8784253
52	10362	965.0646593
53	10326	968.4292078
54	10324	968.6168152
55	10322	968.8044953
56	10320	968.9922481
57	10318	969.1800737
58	10300	970.8737864
59	10280	972.7626459
60	10276	973.1413001
61	10252	975.4194304
62	10228	977.7082519
63	10226	977.8994719
64	10224	978.0907668
65	10128	987.3617694
66	10100	990.0990099
67	10058	994.233446
68	9992	1000.800641
69	9980	1002.004008
70	9938	1006.23868
71	9936	1006.441224
72	9854	1014.816318
73	9826	1017.708121
74	9824	1017.915309
75	9822	1018.122582
76	9674	1033.698573
77	9672	1033.912324
78	9670	1034.126163
79	9668	1034.340091
80	9578	1044.059303
81	9576	1044.27736
82	9574	1044.495509
83	9448	1058.425064
84	9318	1073.191672

Table S1 (continued)

Number	Selected Wavenumber (cm-1)	Corresponding Wavelength (nm)
85	9316	1073.42207
86	9294	1075.962987
87	9292	1076.194576
88	9234	1082.954299
89	9138	1094.331364
90	9136	1094.570928
91	9134	1094.810598
92	9132	1095.050372
93	9130	1095.290252
94	9104	1098.418278
95	8912	1122.082585
96	8910	1122.334456
97	8908	1122.586439
98	8672	1153.136531
99	8670	1153.402537
100	8668	1153.668666
101	8666	1153.934918
102	7974	1254.075746
103	7972	1254.390366
104	7970	1254.705144
105	7968	1255.02008
106	7770	1287.001287
107	7682	1301.744337
108	7680	1302.083333
109	7678	1302.422506
110	7230	1383.125864
111	7228	1383.508578
112	7218	1385.425326
113	7184	1391.982183
114	7182	1392.369813
115	7164	1395.86823
116	7162	1396.258028
117	7160	1396.648045
118	7120	1404.494382
119	7118	1404.889014
120	7104	1407.657658
121	7058	1416.831964
122	7028	1422.879909
123	7026	1423.284942
124	7020	1424.501425
125	7018	1424.907381
126	7002	1428.163382

Table S1 (continued)

Number	Selected Wavenumber (cm-1)	Corresponding Wavelength (nm)
127	7000	1428.571429
128	6984	1431.844215
129	6982	1432.254368
130	6834	1463.271876
131	6818	1466.705779
132	6816	1467.13615
133	6814	1467.566774
134	6772	1476.668636
135	6770	1477.104874
136	6748	1481.920569
137	6704	1491.646778
138	6684	1496.110114
139	6682	1496.557917
140	6674	1498.351813
141	6672	1498.800959
142	6644	1505.117399
143	6642	1505.570611
144	6640	1506.024096
145	6622	1510.117789
146	6620	1510.574018
147	6532	1530.924679
148	6530	1531.393568
149	6500	1538.461538
150	6498	1538.935057
151	6496	1539.408867
152	6472	1545.117429
153	6470	1545.595054
154	6186	1616.553508
155	6184	1617.076326
156	5928	1686.909582
157	5926	1687.478907
158	5560	1798.561151
159	5520	1811.594203
160	5448	1835.535977
161	5446	1836.210062
162	5374	1860.811314
163	5372	1861.504095
164	5370	1862.197393
165	5344	1871.257485
166	5342	1871.958068
167	5336	1874.062969
168	5334	1874.765654

Table S1 (continued)

Number	Selected Wavenumber (cm-1)	Corresponding Wavelength (nm)
169	5332	1875.468867
170	5320	1879.699248
171	5318	1880.406168
172	5316	1881.113619
173	5294	1888.930865
174	5292	1889.644747
175	5252	1904.036558
176	5244	1906.941266
177	5242	1907.668829
178	5228	1912.777353
179	5172	1933.488012
180	5170	1934.235977
181	5048	1980.982567
182	5034	1986.491855
183	5032	1987.281399
184	5024	1990.44586
185	5022	1991.23855
186	5008	1996.805112
187	4978	2008.838891
188	4976	2009.646302
189	4938	2025.111381
190	4936	2025.931929
191	4928	2029.220779
192	4926	2030.044661
193	4924	2030.869212
194	4902	2039.98368
195	4900	2040.816327
196	4892	2044.15372
197	4874	2051.702913
198	4872	2052.545156
199	4858	2058.460272
200	4856	2059.308072
201	4854	2060.156572
202	4782	2091.17524
203	4756	2102.607233
204	4754	2103.491796
205	4752	2104.377104
206	4676	2138.579983
207	4674	2139.495079
208	4668	2142.245073
209	4666	2143.163309
210	4664	2144.082333
211	4630	2159.827214

Table S1 (continued)

Number	Selected Wavenumber (cm-1)	Corresponding Wavelength (nm)
212	4614	2167.316862
213	4612	2168.256722
214	4610	2169.197397
215	4608	2170.138889
216	4606	2171.081198
217	4604	2172.024327
218	4602	2172.968275
219	4600	2173.913043
220	4590	2178.649237
221	4588	2179.598954
222	4520	2212.389381
223	4438	2253.267237
224	4436	2254.283138
225	4434	2255.299955
226	4432	2256.31769
227	4424	2260.39783
228	4422	2261.420172
229	4420	2262.443439
230	4406	2269.63232
231	4404	2270.663034
232	4372	2287.282708
233	4370	2288.329519
234	4368	2289.377289
235	4366	2290.426019
236	4322	2313.743637
237	4320	2314.814815
238	4294	2328.830927
239	4292	2329.916123
240	4272	2340.82397
241	4270	2341.920375
242	4262	2346.316283
243	4260	2347.41784
244	4258	2348.520432
245	4238	2359.603587
246	4236	2360.717658
247	4214	2373.04224
248	4204	2378.686965
249	4196	2383.222116
250	4186	2388.915432
251	4152	2408.477842
252	4144	2413.127413
253	4132	2420.135528
254	4124	2424.830262
255	4090	2444.987775
256	4070	2457.002457
257	4052	2467.917078
258	4000	2500

Table S2. Preliminary comparison of treatment-stage-inclusive feature combinations under MultiScaleSE-GatedCNN.

Group	Baseline feature combination	Treatment-stage-inclusive combination	Baseline Rp2	Baseline RMSEP (mg/L)	Baseline RPD	With treatment stage Rp2	With treatment stage RMSEP (mg/L)	With treatment stage RPD	ΔRp2
G1	Spectra + farm name + longitude + latitude + season	Spectra + farm name + longitude + latitude + treatment stage + season	0.875	421.576	2.825	0.872	426.690	2.792	-0.0031
G2	Spectra + farm name + longitude + season	Spectra + farm name + longitude + treatment stage + season	0.905	367.389	3.242	0.892	391.733	3.041	-0.0130
G3	Spectra + farm name + latitude + season	Spectra + farm name + latitude + treatment stage + season	0.901	374.007	3.185	0.885	403.794	2.950	-0.0163