a

a₁ - Raw spectra
a₂ - ABS spectra
a₃ - KM spectra
a₄ - NOR spectra
a₅ - MSC spectra
a₆ - BC spectra
a₇ - SNV spectra
a₈ - MAS spectra
a₉ - SGS spectra
a₁₀ - MFS spectra
a₁₁ - GFS spectra
a₁₂ - MC spectra
a₁₃ - SG-1D spectra
a₁₄ - SG-2D spectra
a₁₅ - DT spectra
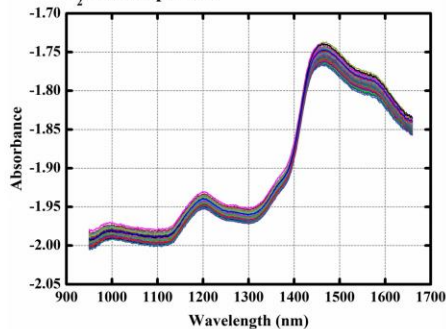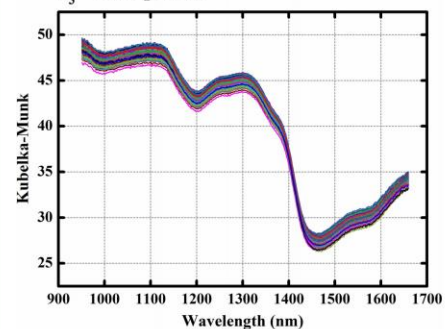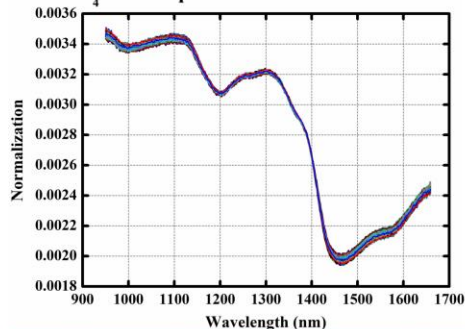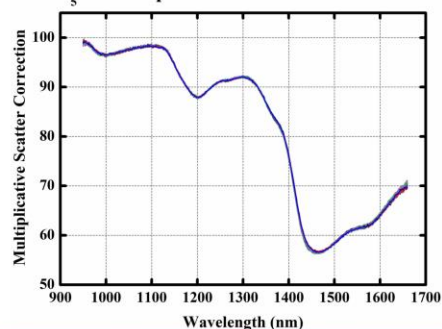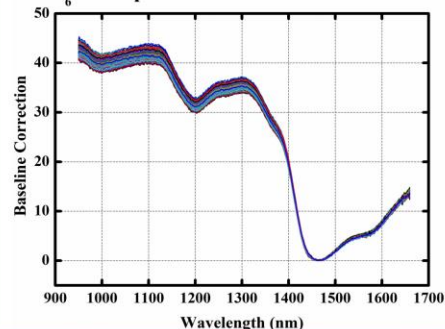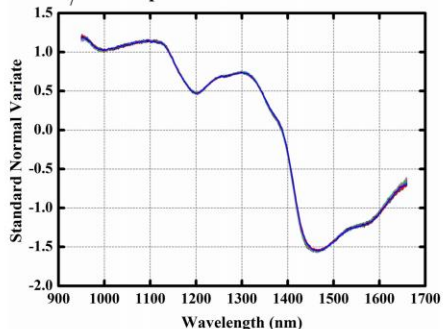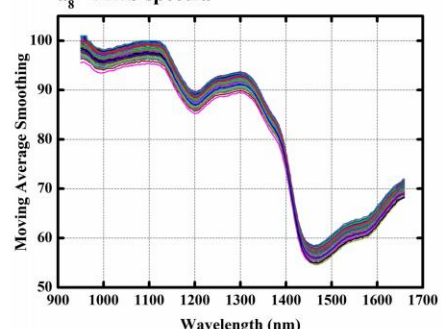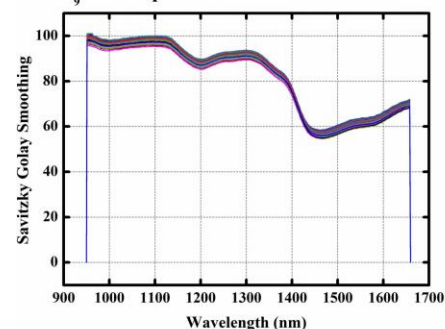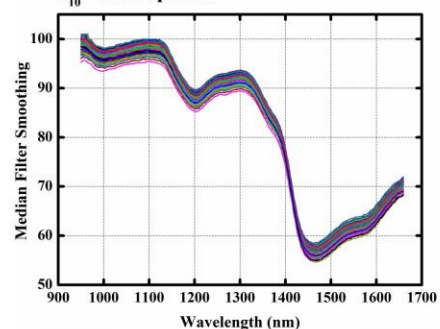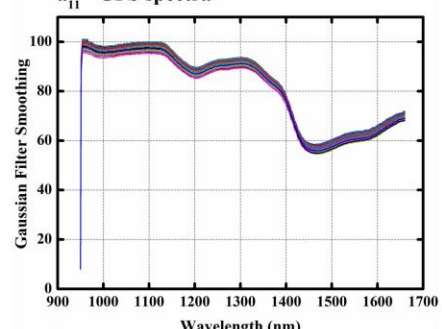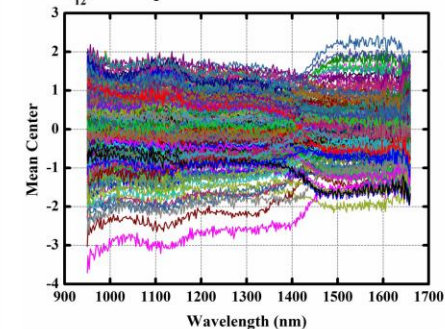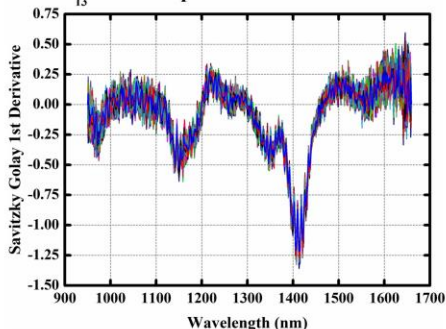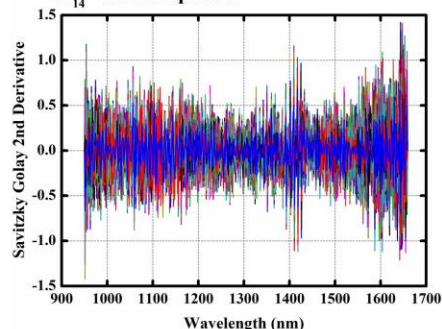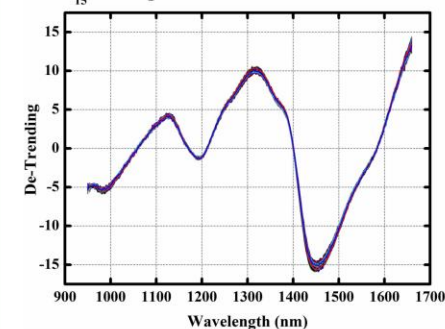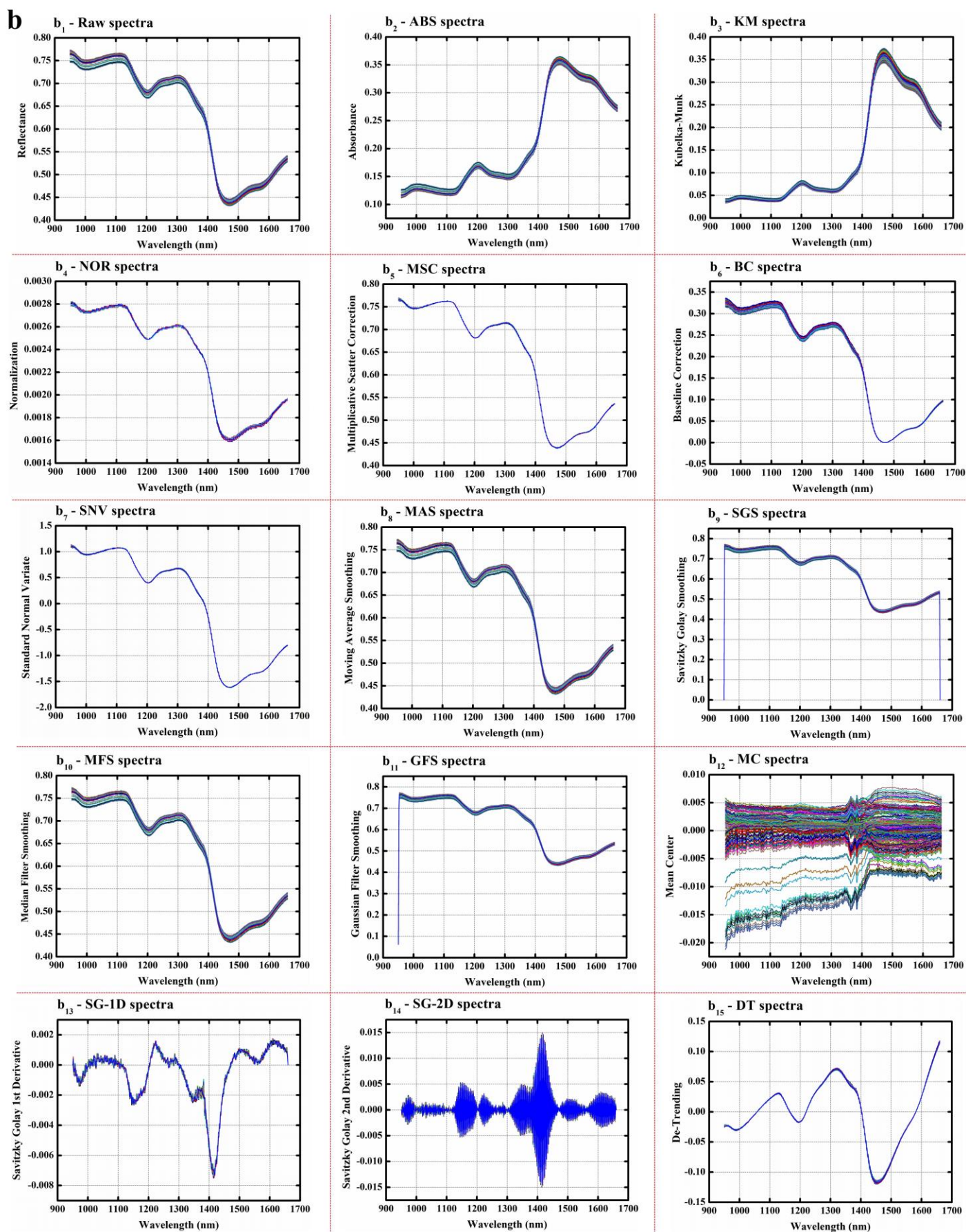
Figure S1. The preprocessed spectral features of all WF samples acquired from NIR device (a) and HSI system (b), respectively.

Table S1: Performances of PLS models for predicting ADA levels (mg/kg) and PLS-DA models for identifying WF samples using full 950–1660 nm spectra from NIR device and from HSI system, based on different numbers of WF samples in training set and validation set, respectively.

NIR source ($N_{T/V}$ group)	Preprocessed spectra	Number of wavelengths	Modeling algorithm	*Quantitative Analysis (determine ADA levels in WF samples)*							*Discriminant Analysis (whether WF samples contain excess ADA)*						
				LVs	R^2_T	$RMSE_T$	R^2_V	$RMSE_V$	RPD	Bias	LVs	R^2_T	$RMSE_T$	AOC	R^2_V	$RMSE_V$	AOC
NIR ($N_{T/V}$=189/21)	RAW	355	PLS	8	0.9823	4.03	0.9737	4.91	6.1754	-0.1891	8	0.9842	0.13	99.47%	0.9698	0.17	100%
	ABS	355	PLS	8	0.9840	3.83	0.9758	4.72	6.4310	-0.2524	8	0.9864	0.12	99.47%	0.9785	0.15	100%
	KM	355	PLS	8	0.9823	4.03	0.9737	4.91	6.1753	-0.1891	8	0.9842	0.13	99.47%	0.9698	0.17	100%
	NOR	355	PLS	8	0.9864	3.53	0.9782	4.47	6.7739	-0.1898	7	0.9828	0.13	99.47%	0.9706	0.18	100%
	MSC	355	PLS	8	0.9909	2.89	0.9866	3.50	8.6559	-0.1106	8	0.9907	0.096	100%	0.9828	0.13	100%
	BC	355	PLS	8	0.9874	3.40	0.9818	4.08	7.4621	-0.2245	8	0.9892	0.10	100%	0.9811	0.14	100%
	SNV	355	PLS	8	0.9909	2.89	0.9866	3.50	8.6556	-0.1109	8	0.9907	0.096	100%	0.9828	0.13	100%
	MAS	355	PLS	10	0.9883	3.28	0.9845	3.77	8.0253	0.1305	10	0.9887	0.11	100%	0.9854	0.12	100%
	SGS	355	PLS	10	0.9887	3.22	0.9858	3.60	8.4093	0.1423	10	0.9886	0.11	100%	0.9843	0.13	100%
	MFS	355	PLS	10	0.9908	2.90	0.9896	3.08	9.8251	-0.08181	10	0.9895	0.10	100%	0.9879	0.11	100%
	GFS	355	PLS	10	0.9953	2.08	0.9933	2.47	12.2907	-0.2333	9	0.9878	0.11	99.47%	0.9805	0.14	100%
	MC	355	PLS	8	0.9822	4.04	0.9736	4.92	6.1558	-0.09857	8	0.9842	0.13	99.47%	0.9698	0.17	100%
	SG1D	**355**	**PLS**	**6**	**0.9864**	**3.54**	**0.9844**	**3.79**	**8.0624**	**0.4845**	**6**	**0.9875**	**0.11**	**99.47%**	**0.9789**	**0.15**	**100%**
	SG2D	355	PLS	5	0.9783	4.46	0.9703	5.22	5.8644	-0.7775	6	0.9864	0.12	100%	0.9827	0.13	100%
	DT	355	PLS	8	0.9916	2.77	0.9870	3.45	8.7941	0.1494	7	0.9864	0.12	100%	0.9763	0.15	100%
NIR ($N_{T/V}$=168/42)	RAW	355	PLS	8	0.9821	4.05	0.9812	4.15	7.3018	0.1084	8	0.9841	0.13	99.47%	0.9799	0.14	100%
	ABS	355	PLS	8	0.9834	3.90	0.9808	4.19	7.2218	0.1455	8	0.9862	0.12	99.47%	0.9838	0.13	100%
	KM	355	PLS	8	0.9821	4.05	0.9812	4.15	7.3018	0.1079	8	0.9841	0.13	99.47%	0.9799	0.14	100%
	NOR	355	PLS	8	0.9864	3.53	0.9849	3.72	8.1416	0.1554	8	0.9883	0.11	99.47%	0.9849	0.12	100%
	MSC	355	PLS	8	0.9907	2.92	0.9891	3.16	9.5881	0.0115	8	0.9907	0.096	99.47%	0.9875	0.11	100%
	BC	355	PLS	8	0.9871	3.43	0.9858	3.61	8.4095	0.2030	8	0.9893	0.10	99.47%	0.9864	0.12	100%
	SNV	355	PLS	8	0.9907	2.92	0.9891	3.16	9.5874	0.01191	8	0.9907	0.096	99.47%	0.9875	0.11	100%
	MAS	355	PLS	10	0.9883	3.27	0.9870	3.45	8.8342	0.3659	10	0.9888	0.11	100%	0.9878	0.11	100%
	SGS	355	PLS	10	0.9888	3.20	0.9881	3.31	9.2066	0.3523	10	0.9887	0.11	100%	0.9872	0.11	100%
	MFS	355	PLS	10	0.9902	3.00	0.9904	2.97	10.2025	0.06437	10	0.9891	0.10	99.47%	0.9894	0.10	100%
	GFS	355	PLS	10	0.9950	2.13	0.9943	2.28	13.2921	-0.1364	10	0.9937	0.079	100%	0.9924	0.087	100%
	MC	355	PLS	8	0.9821	4.05	0.9812	4.15	7.3018	0.1078	8	0.9841	0.13	99.47%	0.9799	0.14	100%
	SG1D	**355**	**PLS**	**6**	**0.9854**	**3.66**	**0.9844**	**3.78**	**8.0048**	**0.07787**	**6**	**0.9866**	**0.12**	**99.47%**	**0.9838**	**0.13**	**100%**
	SG2D	355	PLS	5	0.9778	4.51	0.9755	4.74	6.4193	-0.4186	5	0.9766	0.15	99.47%	0.9730	0.16	100%
	DT	355	PLS	7	0.9861	3.58	0.9858	3.61	8.3900	-0.09138	7	0.9831	0.13	100%	0.9809	0.14	100%
NIR ($N_{T/V}$=147/63)	RAW	355	PLS	8	0.9849	3.72	0.9716	5.10	5.9333	0.1161	8	0.9837	0.13	100%	0.9692	0.18	100%
	ABS	355	PLS	8	0.9846	3.76	0.9725	5.02	6.0287	0.1442	8	0.9842	0.13	100%	0.9690	0.18	100%
	KM	355	PLS	8	0.9849	3.72	0.9716	5.10	5.9332	0.1160	8	0.9837	0.13	100%	0.9692	0.18	100%
	NOR	355	PLS	7	0.9828	3.97	0.9703	5.22	5.8028	0.09055	8	0.9878	0.11	100%	0.9764	0.15	100%
	MSC	355	PLS	6	0.9734	4.93	0.9621	5.90	5.1349	-0.04846	7	0.9863	0.12	99.47%	0.9778	0.15	100%
	BC	355	PLS	8	0.9886	3.24	0.9730	4.97	6.0900	0.1450	8	0.9889	0.11	100%	0.9778	0.15	100%

Group	Method			LV	R²	RMSE	R²	RMSE			LV	R²			R²		
	SNV	355	PLS	6	0.9734	4.93	0.9621	5.90	5.1346	-0.04866	7	0.9863	0.12	99.47%	0.9778	0.15	100%
	MAS	355	PLS	10	0.9882	3.29	0.9677	5.44	5.5726	0.2368	10	0.9886	0.11	100%	0.9779	0.15	100%
	SGS	355	PLS	10	0.9883	3.28	0.9672	5.48	5.5328	0.2780	10	0.9884	0.11	100%	0.9779	0.15	100%
	MFS	355	PLS	10	0.9909	2.89	0.9703	5.22	5.8030	0.1252	10	0.9898	0.10	100%	0.9765	0.15	100%
	GFS	355	PLS	9	0.9895	3.10	0.9759	4.70	6.4618	0.3947	10	0.9942	0.08	100%	0.9849	0.12	100%
	MC	355	PLS	8	0.9849	3.72	0.9716	5.10	5.9333	0.1162	8	0.9837	0.13	100%	0.9692	0.18	100%
	SG1D	**355**	**PLS**	**6**	**0.9872**	**3.43**	**0.9770**	**4.59**	**6.6249**	**0.4254**	**6**	**0.9877**	**0.11**	**100%**	**0.9817**	**0.14**	**100%**
	SG2D	355	PLS	6	0.9875	3.38	0.9729	4.99	6.0902	0.4144	5	0.9750	0.16	99.47%	0.9641	0.19	100%
	DT	355	PLS	7	0.9865	3.52	0.9627	5.85	5.1925	0.4766	8	0.9905	0.10	100%	0.9767	0.15	100%
NIR (N$_{T/V}$=126/84)	RAW	355	PLS	8	0.9845	3.77	0.9775	4.54	6.6686	-0.1240	8	0.9868	0.11	100%	0.9727	0.17	100%
	ABS	355	PLS	8	0.9853	3.67	0.9825	4.01	7.5585	0.05203	8	0.9887	0.11	100%	0.9728	0.16	100%
	KM	355	PLS	8	0.9845	3.77	0.9775	4.54	6.6683	-0.1238	8	0.9868	0.11	100%	0.9727	0.17	100%
	NOR	355	PLS	8	0.9921	2.69	0.9821	4.05	7.4991	-0.2808	8	0.9925	0.09	100%	0.9751	0.16	100%
	MSC	355	PLS	8	0.9922	2.68	0.9790	4.39	6.9510	-0.5660	8	0.9923	0.09	100%	0.9821	0.13	100%
	BC	355	PLS	8	0.9899	3.05	0.9814	4.13	7.3834	-0.5114	8	0.9914	0.09	100%	0.9772	0.15	100%
	SNV	355	PLS	8	0.9922	2.68	0.9790	4.39	6.9511	-0.5663	8	0.9923	0.09	100%	0.9821	0.13	100%
	MAS	355	PLS	10	0.9890	3.17	0.9841	3.82	7.9743	-0.4212	10	0.9887	0.11	100%	0.9679	0.16	100%
	SGS	355	PLS	10	0.9896	3.09	0.9856	3.64	8.3944	-0.4758	10	0.9888	0.11	100%	0.9762	0.15	100%
	MFS	355	PLS	10	0.9915	2.79	0.9826	4.00	7.5762	-0.01752	10	0.9887	0.11	100%	0.9746	0.16	100%
	GFS	355	PLS	10	0.9948	2.19	0.9859	3.59	8.5096	-0.4838	9	0.9895	0.10	100%	0.9713	0.17	100%
	MC	355	PLS	8	0.9845	3.77	0.9775	4.54	6.6686	-0.1237	8	0.9868	0.11	100%	0.9727	0.17	100%
	SG1D	**355**	**PLS**	**6**	**0.9921**	**2.69**	**0.9835**	**3.88**	**7.8415**	**-0.4188**	**6**	**0.9924**	**0.09**	**100%**	**0.9898**	**0.10**	**100%**
	SG2D	355	PLS	5	0.9800	4.28	0.9654	5.63	5.3773	-0.1017	6	0.9874	0.11	100%	0.9800	0.14	100%
	DT	355	PLS	8	0.9937	2.40	0.9882	3.29	9.2508	-0.2911	7	0.9884	0.11	100%	0.9727	0.17	100%
NIR (N$_{T/V}$=105/105)	RAW	355	PLS	8	0.9846	3.76	0.9692	5.31	5.7103	-0.2922	8	0.9838	0.13	99.47%	0.9697	0.17	100%
	ABS	355	PLS	8	0.9867	3.50	0.9737	4.91	6.1879	-0.3982	8	0.9856	0.12	99.47%	0.9823	0.13	100%
	KM	355	PLS	8	0.9846	3.76	0.9692	5.31	5.7101	-0.2922	8	0.9838	0.13	99.47%	0.9697	0.17	100%
	NOR	355	PLS	6	0.9710	5.16	0.9511	6.69	4.5312	-0.3932	7	0.9823	0.13	99.47%	0.9675	0.18	100%
	MSC	355	PLS	8	0.9905	2.95	0.9808	4.19	7.2314	-0.2443	8	0.9901	0.10	99.47%	0.9804	0.14	100%
	BC	355	PLS	7	0.9828	3.97	0.9657	5.61	5.4123	-0.3767	7	0.9808	0.14	99.47%	0.9851	0.12	100%
	SNV	355	PLS	8	0.9905	2.95	0.9808	4.19	7.2315	-0.2446	8	0.9901	0.10	99.47%	0.9804	0.14	100%
	MAS	355	PLS	9	0.9800	4.28	0.9570	6.28	4.8383	-0.5383	11	0.9939	0.08	99.47%	0.9881	0.11	100%
	SGS	355	PLS	7	0.9635	5.78	0.9439	7.17	4.2280	-0.4095	11	0.9941	0.08	99.47%	0.9882	0.11	100%
	MFS	355	PLS	7	0.9621	5.90	0.9446	7.13	4.2591	-0.4876	11	0.9955	0.07	99.47%	0.9897	0.10	100%
	GFS	355	PLS	8	0.9824	4.02	0.9667	5.53	5.4911	-0.3732	10	0.9929	0.08	99.47%	0.9860	0.12	100%
	MC	355	PLS	8	0.9848	3.73	0.9705	5.20	5.8330	-0.2483	8	0.9838	0.13	99.47%	0.9697	0.17	100%
	SG1D	**355**	**PLS**	**6**	**0.9896**	**3.08**	**0.9825**	**4.01**	**7.5584**	**0.1097**	**6**	**0.9894**	**0.10**	**99.47%**	**0.9786**	**0.15**	**100%**
	SG2D	355	PLS	5	0.9790	4.39	0.9635	5.79	5.2385	-0.2815	5	0.9797	0.14	99.47%	0.9605	0.20	100%
	DT	355	PLS	8	0.9927	2.59	0.9862	3.56	8.5107	-0.1768	7	0.9870	0.11	99.47%	0.9754	0.16	100%
HSI-NIR (N$_{T/V}$=189/21)	**RAW**	**432**	**PLS**	**9**	**0.9850**	**3.70**	**0.9872**	**3.43**	**8.8350**	**-0.1358**	**11**	**0.9809**	**0.14**	**100%**	**0.9629**	**0.19**	**100%**
	ABS	432	PLS	9	0.9832	3.92	0.9836	3.87	7.8201	-0.08105	11	0.9797	0.14	100%	0.9584	0.20	100%
	KM	432	PLS	9	0.9843	3.80	0.9796	4.32	7.0308	-0.3899	11	0.9692	0.18	100%	0.9359	0.25	100%
	NOR	432	PLS	8	0.9820	4.07	0.9802	4.26	7.1594	0.5126	11	0.9832	0.13	100%	0.9628	0.19	100%
	MSC	432	PLS	7	0.9784	4.45	0.9744	4.85	6.2492	-0.1931	10	0.9825	0.13	100%	0.9627	0.19	100%

BC	432	PLS	9	0.9897	3.07	0.9867	3.49	8.6689	-0.05602	11	0.9763	0.15	100%	0.9503	0.22	100%
SNV	432	PLS	7	0.9784	4.45	0.9743	4.85	6.2487	-0.1929	10	0.9825	0.13	100%	0.9627	0.19	100%
MAS	432	PLS	9	0.9824	4.01	0.9845	3.76	8.0486	-0.1124	11	0.9712	0.17	100%	0.9403	0.24	100%
SGS	432	PLS	9	0.9826	3.99	0.9845	3.77	8.0398	-0.1334	11	0.9719	0.17	100%	0.9399	0.24	100%
MFS	432	PLS	9	0.9839	3.84	0.9858	3.61	8.4089	-0.2015	11	0.9767	0.15	100%	0.9507	0.22	100%
GFS	432	PLS	9	0.9843	3.80	0.9863	3.54	8.5676	-0.1603	11	0.9797	0.14	100%	0.9589	0.20	100%
MC	432	PLS	9	0.9850	3.70	0.9872	3.43	8.8350	-0.1356	11	0.9809	0.14	100%	0.9629	0.19	100%
SG1D	432	PLS	6	0.9768	4.62	0.9712	5.13	5.9028	-0.07497	6	0.9538	0.21	100%	0.9250	0.27	100%
SG2D	432	PLS	6	0.9771	4.58	0.9734	4.94	6.1333	0.03004	6	0.9532	0.22	100%	0.9309	0.26	100%
DT	432	PLS	6	0.9668	5.52	0.9601	6.05	5.0104	0.1992	10	0.9785	0.15	100%	0.9485	0.23	100%
RAW	**432**	**PLS**	**9**	**0.9850**	**3.71**	**0.9876**	**3.37**	**9.0233**	**0.3178**	**11**	**0.9811**	**0.14**	**100%**	**0.9661**	**0.18**	**100%**
ABS	432	PLS	9	0.9830	3.94	0.9851	3.69	8.2217	0.2874	11	0.9805	0.14	100%	0.9709	0.17	100%
KM	432	PLS	9	0.9839	3.85	0.9832	3.92	7.7332	-0.2408	11	0.9703	0.17	100%	0.9417	0.24	100%
NOR	432	PLS	8	0.9811	4.16	0.9822	4.04	7.5813	0.6350	11	0.9836	0.13	100%	0.9662	0.18	100%
MSC	432	PLS	8	0.9842	3.81	0.9848	3.74	8.1100	0.1688	10	0.9833	0.13	100%	0.9644	0.19	100%
BC	432	PLS	8	0.9799	4.29	0.9816	4.11	7.4746	0.6931	11	0.9765	0.15	99.40%	0.9689	0.18	100%
HSI-NIR ($N_{T/V}$=168/42) SNV	432	PLS	8	0.9842	3.81	0.9848	3.74	8.1100	0.1684	10	0.9833	0.13	100%	0.9644	0.19	100%
MAS	432	PLS	9	0.9820	4.06	0.9856	3.63	8.4125	0.4613	11	0.9709	0.17	99.40%	0.9557	0.21	100%
SGS	432	PLS	9	0.9823	4.03	0.9858	3.61	8.4620	0.4520	11	0.9717	0.17	99.40%	0.9553	0.21	100%
MFS	432	PLS	9	0.9834	3.90	0.9867	3.50	8.6980	0.3338	11	0.9767	0.15	100%	0.9607	0.20	100%
GFS	432	PLS	9	0.9841	3.82	0.9872	3.43	8.8796	0.3298	11	0.9796	0.14	100%	0.9648	0.19	100%
MC	432	PLS	9	0.9850	3.71	0.9876	3.37	9.0233	0.3177	11	0.9811	0.14	100%	0.9661	0.18	100%
SG1D	432	PLS	6	0.9758	4.71	0.9664	5.55	5.4569	-0.1073	6	0.9552	0.21	99.40%	0.9218	0.28	100%
SG2D	432	PLS	6	0.9763	4.66	0.9671	5.50	5.5097	-0.05720	6	0.9554	0.21	100%	0.9198	0.28	100%
DT	432	PLS	6	0.9658	5.60	0.9684	5.38	5.6561	0.5637	10	0.9786	0.15	99.40%	0.9592	0.20	100%
RAW	**432**	**PLS**	**9**	**0.9847**	**3.75**	**0.9831**	**3.94**	**7.8453**	**0.7764**	**11**	**0.9832**	**0.13**	**100%**	**0.9584**	**0.20**	**100%**
ABS	432	PLS	9	0.9826	3.99	0.9817	4.10	7.5451	0.8256	11	0.9823	0.13	99.32%	0.9785	0.15	100%
KM	432	PLS	9	0.9823	4.03	0.9790	4.39	7.2530	1.3518	11	0.9714	0.17	99.32%	0.9410	0.24	99.32%
NOR	432	PLS	9	0.9829	3.96	0.9842	3.81	8.0341	0.5295	11	0.9857	0.12	100%	0.9597	0.20	100%
MSC	432	PLS	7	0.9850	3.71	0.9834	3.90	7.7958	0.3399	10	0.9847	0.12	100%	0.9593	0.20	100%
BC	432	PLS	8	0.9807	4.20	0.9824	4.01	7.5851	0.4199	12	0.9872	0.11	100%	0.9615	0.20	100%
HSI-NIR ($N_{T/V}$=147/63) SNV	432	PLS	7	0.9850	3.71	0.9834	3.90	7.7958	0.3398	10	0.9847	0.12	100%	0.9593	0.20	100%
MAS	432	PLS	9	0.9829	3.96	0.9816	4.11	7.4460	0.6155	11	0.9742	0.16	99.32%	0.9423	0.24	100%
SGS	432	PLS	9	0.9831	3.94	0.9817	4.10	7.4690	0.5971	11	0.9751	0.16	99.32%	0.9439	0.24	100%
MFS	432	PLS	9	0.9838	3.86	0.9829	3.96	7.7704	0.6996	11	0.9788	0.15	99.32%	0.9483	0.23	100%
GFS	432	PLS	9	0.9841	3.82	0.9824	4.01	3.9814	0.7162	11	0.9819	0.13	100%	0.9557	0.21	100%
MC	432	PLS	9	0.9847	3.75	0.9831	3.94	7.8453	0.7769	11	0.9832	0.13	100%	0.9584	0.20	100%
SG1D	432	PLS	6	0.9778	4.51	0.9709	5.16	6.0000	1.0997	6	0.9503	0.22	100%	0.9343	0.26	100%
SG2D	432	PLS	6	0.9782	4.47	0.9715	5.11	6.1020	1.2128	7	0.9659	0.18	100%	0.9438	0.24	100%
DT	432	PLS	6	0.9660	5.59	0.9681	5.41	5.6013	0.1717	11	0.9901	0.10	100%	0.9584	0.20	100%
RAW	**432**	**PLS**	**9**	**0.9856**	**3.64**	**0.9812**	**4.15**	**7.3107**	**0.2519**	**11**	**0.9825**	**0.13**	**100%**	**0.9426**	**0.24**	**100%**
HSI-NIR ($N_{T/V}$=126/84) ABS	432	PLS	10	0.9927	2.58	0.9869	3.46	8.7585	0.1604	11	0.9812	0.14	100%	0.9721	0.17	100%
KM	432	PLS	9	0.9842	3.81	0.9758	4.71	6.4954	0.7001	10	0.9636	0.19	100%	0.9049	0.31	100%
NOR	432	PLS	8	0.9814	4.13	0.9759	4.70	6.4604	0.2975	10	0.9748	0.16	99.21%	0.9256	0.27	100%

	MSC	432	PLS	8	0.9868	3.48	0.9779	4.50	6.7612	0.4539	10	0.9835	0.13	100%	0.9429	0.24	100%
	BC	432	PLS	8	0.9802	4.26	0.9748	4.80	6.3140	0.3029	10	0.9720	0.17	99.21%	0.9314	0.26	100%
	SNV	432	PLS	8	0.9868	3.48	0.9779	4.50	6.7617	0.4548	10	0.9835	0.13	100%	0.9429	0.24	100%
	MAS	432	PLS	9	0.9825	4.01	0.9792	4.36	6.9549	0.2758	11	0.9720	0.17	100%	0.9251	0.27	100%
	SGS	432	PLS	9	0.9827	3.98	0.9796	4.33	7.0069	0.2699	11	0.9725	0.17	100%	0.9253	0.27	100%
	MFS	432	PLS	9	0.9840	3.83	0.9806	4.22	7.1971	0.2963	11	0.9781	0.15	100%	0.9346	0.26	100%
	GFS	432	PLS	9	0.9846	3.75	0.9807	4.21	7.2039	0.2535	11	0.9809	0.14	100%	0.9401	0.24	100%
	MC	432	PLS	9	0.9856	3.64	0.9812	4.15	7.3107	0.2511	11	0.9825	0.13	100%	0.9426	0.24	100%
	SG1D	432	PLS	5	0.9702	5.22	0.9459	7.04	4.3744	1.2819	7	0.9721	0.17	100%	0.9022	0.31	97.62%
	SG2D	432	PLS	5	0.9703	5.22	0.9466	7.00	4.4085	1.3526	7	0.9732	0.16	100%	0.9010	0.31	97.62%
	DT	432	PLS	6	0.9671	5.49	0.9601	6.05	5.0224	0.4859	10	0.9826	0.13	100%	0.9284	0.27	100%
	RAW	**432**	**PLS**	**8**	**0.9872**	**3.42**	**0.9832**	**3.92**	**7.8392**	**0.6914**	**10**	**0.9876**	**0.11**	**99.05%**	**0.9698**	**0.17**	**100%**
	ABS	432	PLS	9	0.9847	3.74	0.9815	4.12	7.4441	0.6587	11	0.9870	0.11	99.05%	0.9679	0.18	100%
	KM	432	PLS	9	0.9842	3.80	0.9797	4.31	7.0326	0.2698	9	0.9427	0.24	98.10%	0.9186	0.29	100%
	NOR	432	PLS	8	0.9823	4.03	0.9804	4.24	7.1967	0.5368	11	0.9888	0.11	99.05%	0.9684	0.18	100%
	MSC	432	PLS	8	0.9859	3.60	0.9845	3.76	8.1599	0.6431	10	0.9883	0.11	99.05%	0.9688	0.18	100%
	BC	432	PLS	8	0.9820	4.06	0.9806	4.22	7.2681	0.6869	11	0.9841	0.13	99.05%	0.9643	0.19	100%
HSI-NIR	SNV	432	PLS	8	0.9859	3.60	0.9845	3.77	8.1598	0.6417	10	0.9883	0.11	99.05%	0.9688	0.18	100%
($N_{T/V}$=105/105)	MAS	432	PLS	9	0.9840	3.83	0.9808	4.19	7.3590	0.7946	12	0.9858	0.12	99.05%	0.9664	0.18	100%
	SGS	432	PLS	9	0.9843	3.80	0.9813	4.14	7.4451	0.7937	12	0.9859	0.12	99.05%	0.9665	0.18	100%
	MFS	432	PLS	9	0.9855	3.65	0.9820	4.06	7.5820	0.7399	11	0.9815	0.14	99.05%	0.9651	0.19	100%
	GFS	432	PLS	9	0.9872	3.42	0.9832	3.92	7.8392	0.6914	11	0.9876	0.11	99.05%	0.9698	0.17	100%
	MC	432	PLS	9	0.9872	3.42	0.9832	3.92	7.8392	0.6909	11	0.9876	0.11	99.05%	0.9698	0.17	100%
	SG1D	432	PLS	6	0.9792	4.36	0.9701	5.24	5.7799	-0.1184	6	0.9647	0.19	99.05%	0.9284	0.27	100%
	SG2D	432	PLS	6	0.9800	4.28	0.9704	5.21	5.8176	-0.1575	6	0.9645	0.19	99.05%	0.9291	0.27	100%
	DT	432	PLS	8	0.9858	3.61	0.9836	3.88	7.8627	0.4886	10	0.9867	0.12	99.05%	0.9648	0.19	100%

Table S2: The MEWs selected by SRC method from SG1D spectra (originated from NIR) and raw spectra (originated from HSI), respectively.

NIR source ($N_{T/V}$ group)	Preprocessed spectra	MEWs selection Method	Number of MEWs	Specific MEWs	Wavelength reduction
NIR ($N_{T/V}$=189/21)	SG1D	SRC	26	1009.98, 1012.51, 1016.31, 1027.68, 1035.24, 1044.04, 1061.56, 1062.8, 1096.31, 1117.22, 1145.29, 1147.72, 1152.57, 1173.11, 1240.93, 1289.89, 1443.64, 1468.55, 1480.38,1497.47, 1505.97, 1532.34, 1546.97, 1578.00, 1590.29, 1612.64	93%
NIR ($N_{T/V}$=168/42)	**SG1D**	**SRC**	**24**	**989.63, 1009.98, 1016.31, 1044.04, 1047.8, 1052.81, 1156.21, 1173.11, 1206.62, 1240.93, 1242.10, 1281.79, 1295.66, 1335.72, 1343.66, 1407.44, 1443.64, 1445.81, 1468.55, 1480.38, 1485.73, 1513.39, 1570.80, 1608.60**	**93%**
NIR ($N_{T/V}$=147/63)	SG1D	SRC	26	953.72, 1009.98, 1012.51, 1032.72, 1041.53, 1044.04, 1082.7, 1100.01, 1122.12, 1127.01, 1173.11, 1227.96, 1289.89, 1293.35, 1311.76, 1377.43, 1407.44, 1468.55, 1480.38, 1490.01, 1497.47, 1510.21, 1546.97, 1561.51, 1578.00, 1601.50	93%
NIR ($N_{T/V}$=126/84)	SG1D	SRC	30	960.16, 1030.2, 1047.8, 1087.66, 1098.78, 1173.11,1183.92, 1206.62, 1238.58, 1279.47, 1293.35, 1295.66, 1309.46, 1345.93, 1403.01, 1420.66, 1422.86, 1443.64, 1476.08, 1480.38, 1500.66, 1534.44, 1546.97, 1549.05, 1558.40, 1566.68, 1587.23, 1589.27, 1610.62, 1648.71	92%
NIR ($N_{T/V}$=105/105)	SG1D	SRC	22	965.3, 1012.51, 1015.05, 1016.31, 1153.79, 1173.11, 1192.3, 1269.01, 1295.66, 1308.32, 1361.72, 1425.05, 1443.64, 1465.32, 1466.40, 1468.55, 1546.97, 1552.17, 1601.50, 1612.64, 1624.74, 1640.75	94%
HSI-NIR ($N_{T/V}$=189/21)	RAW	SRC	29	949.945, 951.591, 1009.192, 1019.064, 1032.225, 1037.16, 1060.19, 1073.349, 1094.732, 1102.955, 1142.428, 1165.453, 1168.743, 1176.966, 1257.572, 1293.774, 1313.525, 1369.509, 1379.393, 1382.687, 1392.573, 1428.83, 1437.073, 1511.314, 1577.399, 1584.013, 1608.825, 1623.719, 1660.152	93%
HSI-NIR ($N_{T/V}$=168/42)	RAW	SRC	26	949.945, 994.383, 1009.192, 1019.064, 1094.732, 1099.666, 1111.179, 1121.047, 1142.428, 1163.809, 1165.453, 1178.611, 1185.190, 1234.538, 1257.572, 1293.774, 1339.866, 1369.509, 1379.393, 1382.687, 1385.982, 1395.868, 1511.314, 1584.013, 1623.719, 1660.152	94%
HSI-NIR ($N_{T/V}$=147/63)	**RAW**	**SRC**	**23**	**1009.192, 1020.709, 1037.16, 1073.349, 1094.732, 1102.955, 1129.27, 1145.717, 1168.743, 1198.349, 1257.572, 1313.525, 1359.627, 1362.921, 1369.509, 1379.393, 1387.63, 1392.573, 1475.006, 1557.564, 1577.399, 1593.936, 1633.652**	**95%**
HSI-NIR ($N_{T/V}$=126/84)	RAW	SRC	30	949.945, 1004.256, 1035.515, 1102.955, 1106.245, 1158.874, 1165.453, 1168.743, 1244.409, 1257.572, 1270.735, 1277.317, 1300.357, 1326.695, 1333.28, 1343.16, 1369.509, 1372.804, 1382.687, 1387.63, 1392.573, 1521.221, 1537.737, 1567.48, 1593.936, 1597.244, 1623.719, 1633.652, 1640.275, 1660.152	93%
HSI-NIR ($N_{T/V}$=105/105)	RAW	SRC	24	949.945, 1019.064, 1043.741, 1132.56, 1142.428, 1152.296, 1165.453, 1168.743, 1178.611, 1224.668, 1234.538, 1241.119, 1290.482, 1329.988, 1333.28, 1369.509, 1379.393, 1446.966, 1448.615, 1488.206, 1508.012, 1579.052, 1613.789, 1660.152	94%

Table S3: Predicting ADA levels in WF using MEWs based on the different numbers of WF samples in training set and validation set.

NIR source (N_T/V group)	Preprocessed spectra	Number of MEWs	Modeling algorithm	LVs	Quantitative Regression Analysis							Discriminant Analysis (whether excessive ADA)						
					Training set		Validation set				ΔE	LVs	Training set			Validation set		
					R^2_T	$RMSE_T$	R^2_V	$RMSE_V$	RPD	Bias			R^2_T	$RMSE_T$	AOC	R^2_V	$RMSE_V$	AOC
NIR (N_T/V=189/21)	SG1D	26	PLS	5	0.9875	3.38	0.9858	3.61	8.4333	-0.4003	0.23	4	0.9328	0.26	98.41%	0.8917	0.33	95.24%
			MLR	—	0.9908	2.91	0.9891	3.16	9.6827	-0.4378	0.25	—	0.9543	0.21	98.94%	0.9209	0.28	100%
NIR (N_T/V=168/42)	**SG1D**	**24**	PLS	4	0.9810	4.18	0.9819	4.08	7.4889	-0.5363	0.10	3	0.9091	0.30	98.21%	0.9119	0.30	97.62%
			MLR	—	**0.9914**	**2.81**	**0.9898**	**3.06**	**9.9001**	**-0.1769**	**0.25**	—	**0.9410**	**0.24**	**99.40%**	**0.9369**	**0.25**	**100%**
NIR (N_T/V=147/63)	SG1D	26	PLS	5	0.9844	3.78	0.9607	6.00	5.1775	1.3526	2.22	5	0.9333	0.26	97.96%	0.9094	0.30	98.41%
			MLR	—	0.9908	2.90	0.9887	4.70	6.6141	1.0849	1.80	—	0.9509	0.22	99.32%	0.9229	0.28	100%
NIR (N_T/V=126/84)	SG1D	30	PLS	6	0.9894	3.12	0.9839	3.84	7.8833	0.1407	0.72	5	0.9253	0.27	97.62%	0.9344	0.26	98.81%
			MLR	—	0.9947	2.54	0.9907	2.92	10.3561	-0.0071	0.39	—	0.9578	0.21	99.21%	0.9464	0.23	100%
NIR (N_T/V=105/105)	SG1D	22	PLS	5	0.9849	3.72	0.9754	4.74	6.3994	0.3491	1.02	3	0.9109	0.30	99.05%	0.8809	0.34	98.10%
			MLR	—	0.9884	3.26	0.9789	4.40	6.8888	0.1006	1.13	—	0.9458	0.23	99.05%	0.9278	0.27	98.10%
HSI-NIR (N_T/V=189/21)	RAW	29	PLS	9	0.9920	2.71	0.9854	3.66	8.3023	0.2916	0.95	8	0.8985	0.32	96.83%	0.8792	0.35	100%
			MLR	—	0.9944	2.27	0.9848	3.73	8.1736	0.4101	1.45	—	0.9203	0.28	98.94%	0.8585	0.38	100%
HSI-NIR (N_T/V=168/42)	RAW	26	PLS	8	0.9922	2.68	0.9838	3.86	8.0896	0.9310	1.18	8	0.8992	0.32	98.81%	0.8997	0.32	100%
			MLR	—	0.9942	2.31	0.9848	3.74	8.1754	0.5071	1.43	—	0.9157	0.29	100%	0.9018	0.31	100%
HSI-NIR (N_T/V=147/63)	**RAW**	**23**	PLS	7	0.9892	3.15	0.9835	3.88	7.7972	0.1024	0.74	8	0.9038	0.31	98.64%	0.8765	0.35	100%
			MLR	—	**0.9919**	**2.72**	**0.9837**	**3.86**	**7.8388**	**0.0836**	**1.14**	—	**0.9101**	**0.30**	**99.32%**	**0.8787**	**0.35**	**100%**
HSI-NIR (N_T/V=126/84)	RAW	30	PLS	9	0.9923	2.66	0.9801	4.27	7.1218	0.4427	1.62	8	0.8816	0.34	96.03%	0.8517	0.38	96.43%
			MLR	—	0.9937	2.40	0.9795	4.33	7.0018	0.2873	1.93	—	0.9122	0.30	98.41%	0.8354	0.41	97.62%
HSI-NIR (N_T/V=105/105)	RAW	24	PLS	9	0.9913	2.83	0.9825	4.00	7.5800	0.2076	1.17	7	0.8892	0.33	96.19%	0.8860	0.34	97.14%
			MLR	—	0.9944	2.26	0.9827	3.98	7.5990	-0.01286	1.72	—	0.9201	0.28	99.05%	0.8905	0.33	100%