Mellansvensk växtodlingskonferens 19-20 januari 2021

Spectral analysis and multivariate methods for assessing botanical composition in leys

Leonardo A Monteiro

Umeå, 2020

Why to assess leys…

- Importance of clover in grazing systems
- Forage quality and quantity
- Nitrogen management
- Forage botanical composition
- Multivariate analysis - spectral techniques

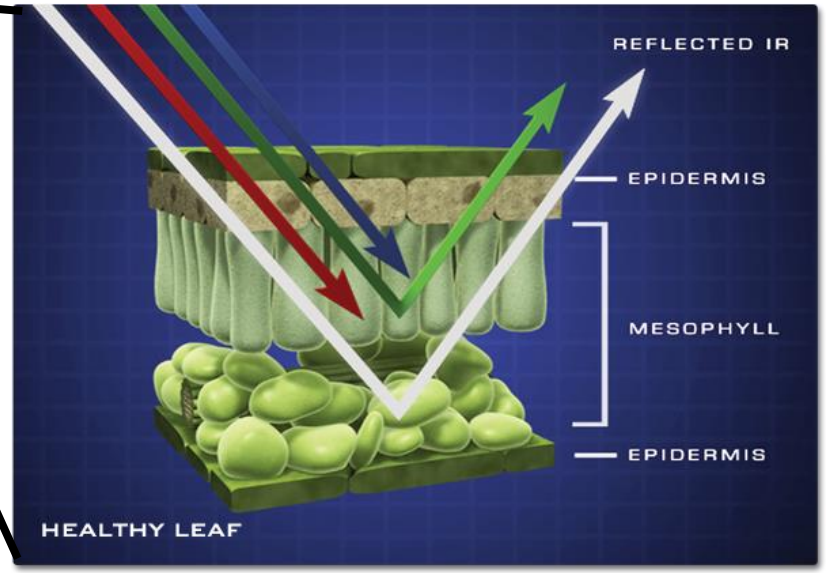
Methodology

- 6 locations

Methodology

- Spectra collected via Hand-held YaraNSensor equipment

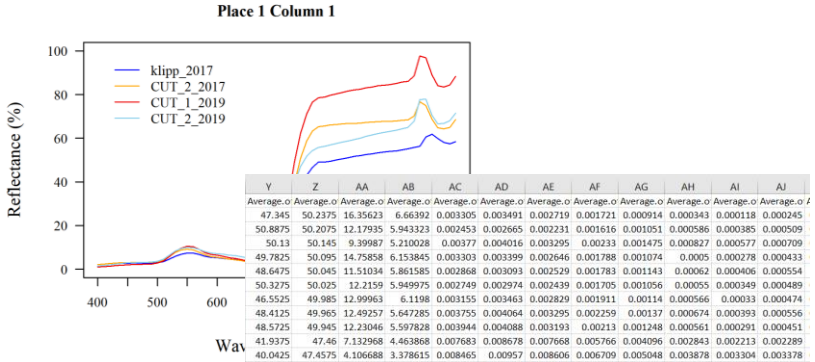
- (vis-NIR 400-1000 nm) – average of 4 measurements (2017 – 2019)



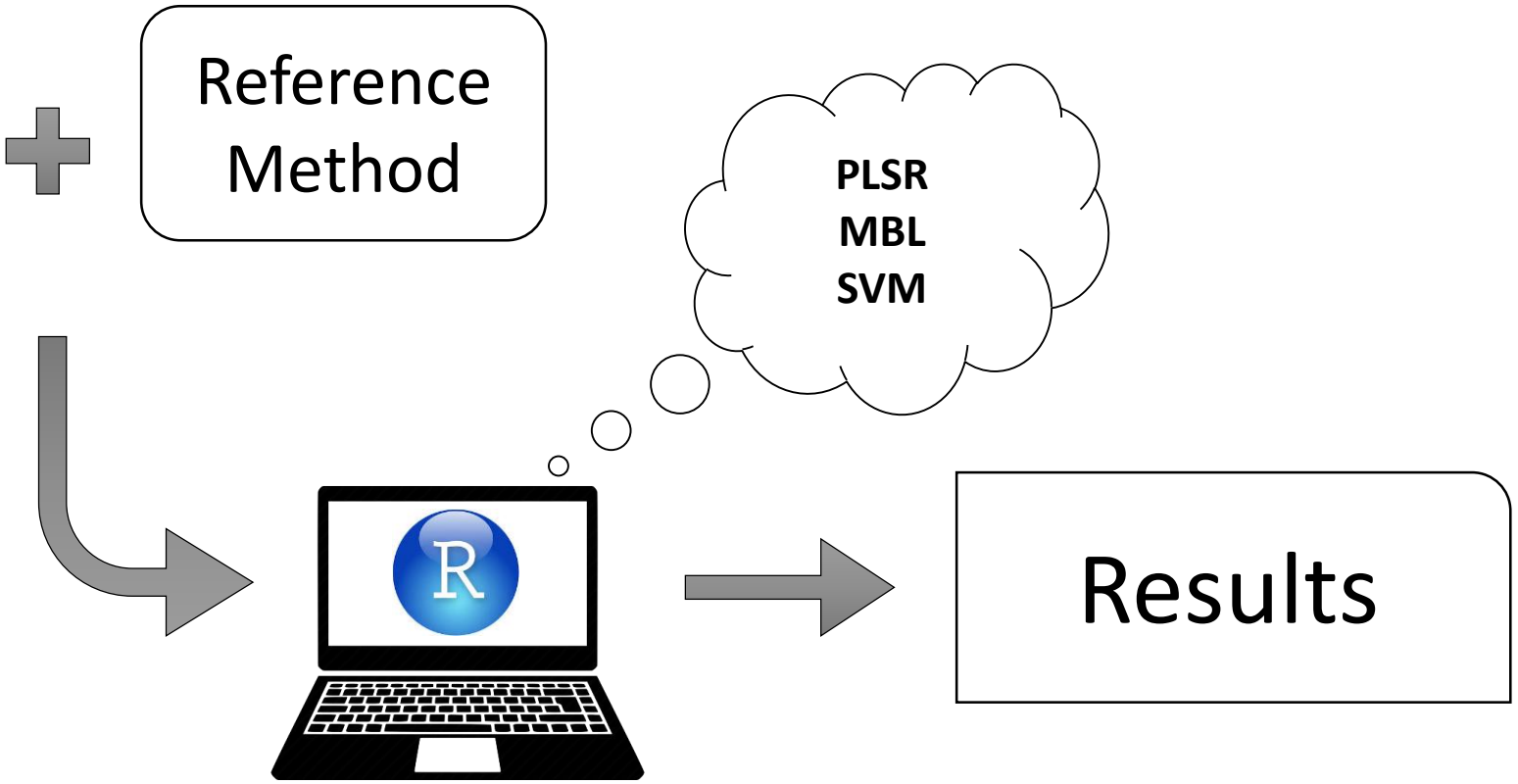
YaraNSensor

Methodology

Multivariate analysis to estimate clover content (indirect)

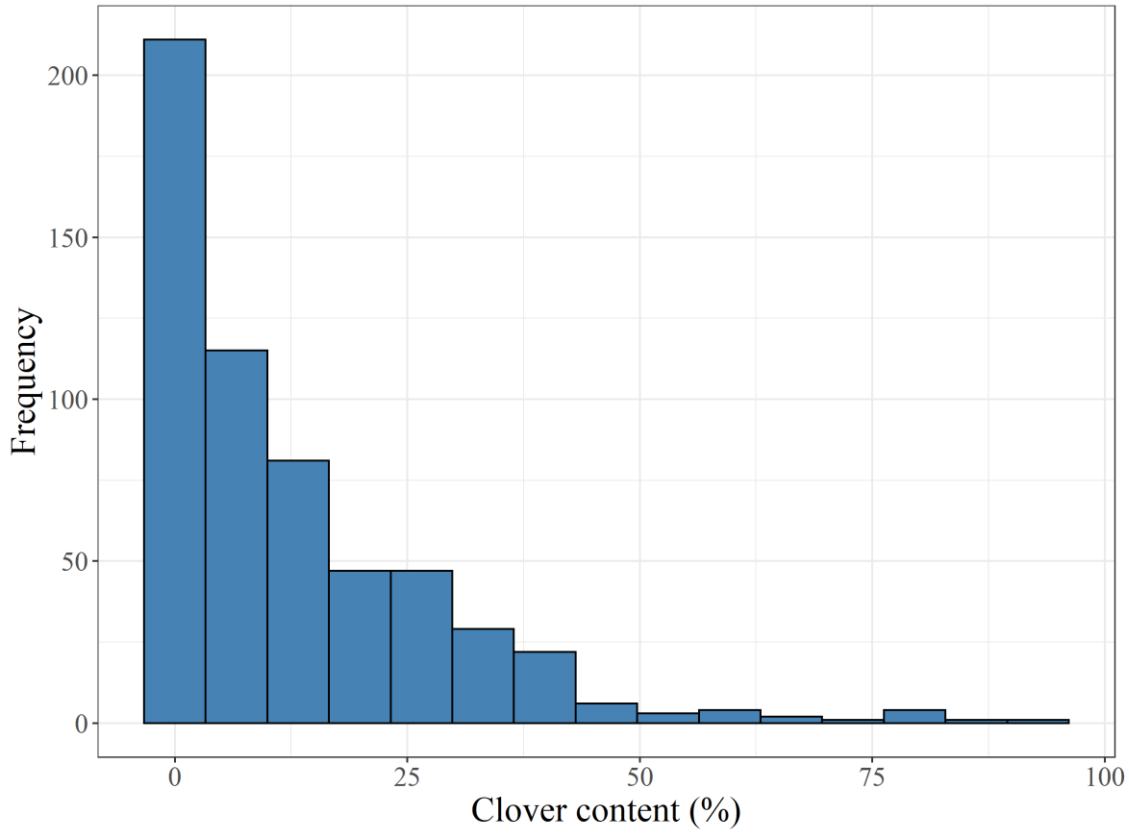


Y	Z	AA	AB	AC	AD	AE	AF	AG	AH	AI	AJ
Average.o	Average.o	Average.o	Average.o	Average.o	Average.o	Average.o	Average.o	Average.o	Average.o	Average.o	Average.o
47.345	50.2375	16.35623	6.66392	0.003305	0.003491	0.002719	0.001721	0.000914	0.000343	0.000118	0.000245
50.8875	50.2075	12.17935	5.943323	0.002453	0.002665	0.002231	0.001616	0.001051	0.000586	0.000385	0.000509
50.13	50.145	9.39987	5.210028	0.00377	0.004016	0.003295	0.00233	0.001475	0.000827	0.000577	0.000709
49.7825	50.095	14.75858	6.153845	0.003303	0.003399	0.002646	0.001788	0.001074	0.0005	0.000278	0.000433
48.6475	50.045	11.51034	5.861585	0.002868	0.003093	0.002529	0.001783	0.001143	0.00062	0.000406	0.000554
50.3275	50.025	12.2159	5.949975	0.002749	0.002974	0.002439	0.001705	0.001056	0.00055	0.000349	0.000489
46.5525	49.985	12.99963	6.1198	0.003155	0.003463	0.002829	0.001911	0.00114	0.000566	0.00033	0.000474
48.4125	49.965	12.49257	5.647285	0.003755	0.004064	0.003295	0.002259	0.00137	0.000674	0.000393	0.000556
48.5725	49.945	12.23046	5.597828	0.003944	0.004088	0.003193	0.00213	0.001248	0.000561	0.000291	0.000451
41.9375	47.46	7.132968	4.463868	0.007683	0.008678	0.007668	0.005766	0.004096	0.002843	0.002213	0.002289
40.0425	47.4575	4.106688	3.378615	0.008465	0.00957	0.008606	0.006709	0.005048	0.003878	0.003304	0.003378
42.3425	47.465	6.795253	4.627815	0.00745	0.008219	0.007163	0.005383	0.003875	0.002753	0.002191	0.002279
61.6225	47.4925	7.068243	4.748428	0.006964	0.007543	0.006535	0.004993	0.003653	0.002641	0.002158	0.002229
57.805	47.4975	4.56511	3.605343	0.007605	0.008524	0.0076	0.005928	0.004491	0.003441	0.002904	0.002975
60.3275	47.4975	6.264575	4.367325	0.00725	0.008119	0.007146	0.005441	0.003985	0.002881	0.002325	0.002415
62.705	47.4975	7.932775	4.947863	0.006939	0.007616	0.006536	0.004813	0.003376	0.002314	0.001781	0.001869
43.535	47.4975	3.96219	3.377458	0.007579	0.008505	0.007633	0.006001	0.004596	0.003598	0.003098	0.00315
43.86	47.4975	6.318328	4.388618	0.00689	0.007704	0.006784	0.005165	0.003774	0.002738	0.002218	0.002308
5.4225	24.71	19.38331	6.330513	0.005124	0.00598	0.004943	0.003183	0.001804	0.000813	0.000227	0.000424

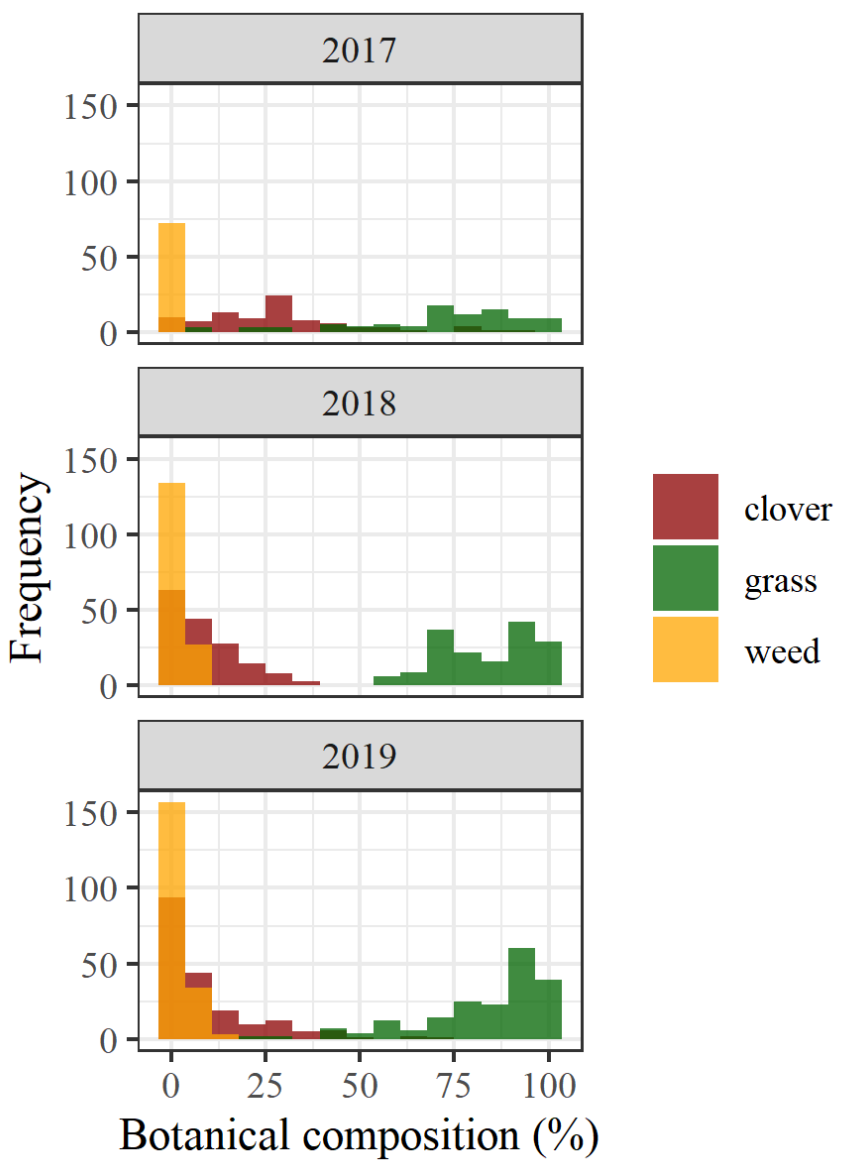


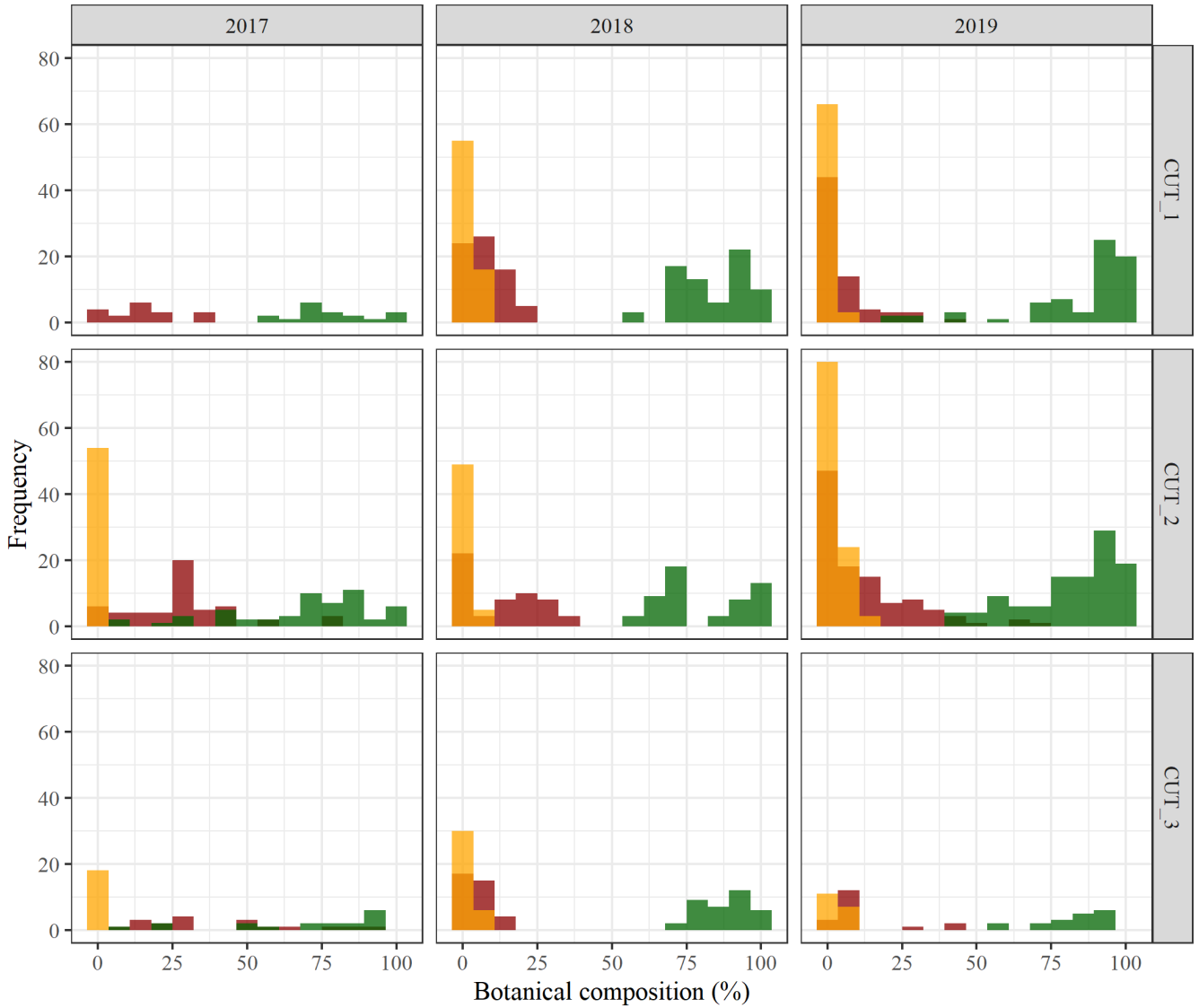
Exploring the data

- Clover content distribution



Variation in botanical composition





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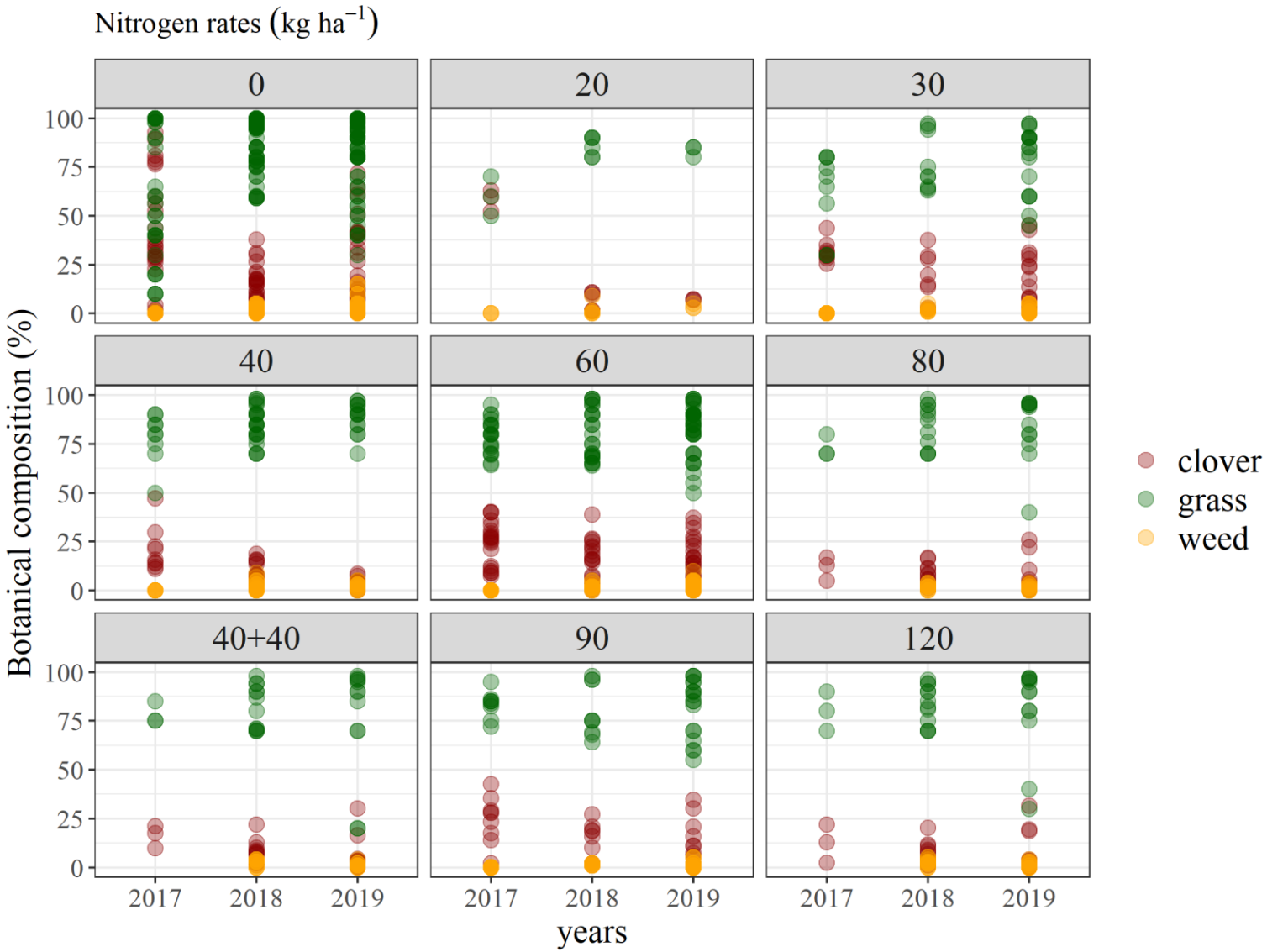


Match the spectra with reference method

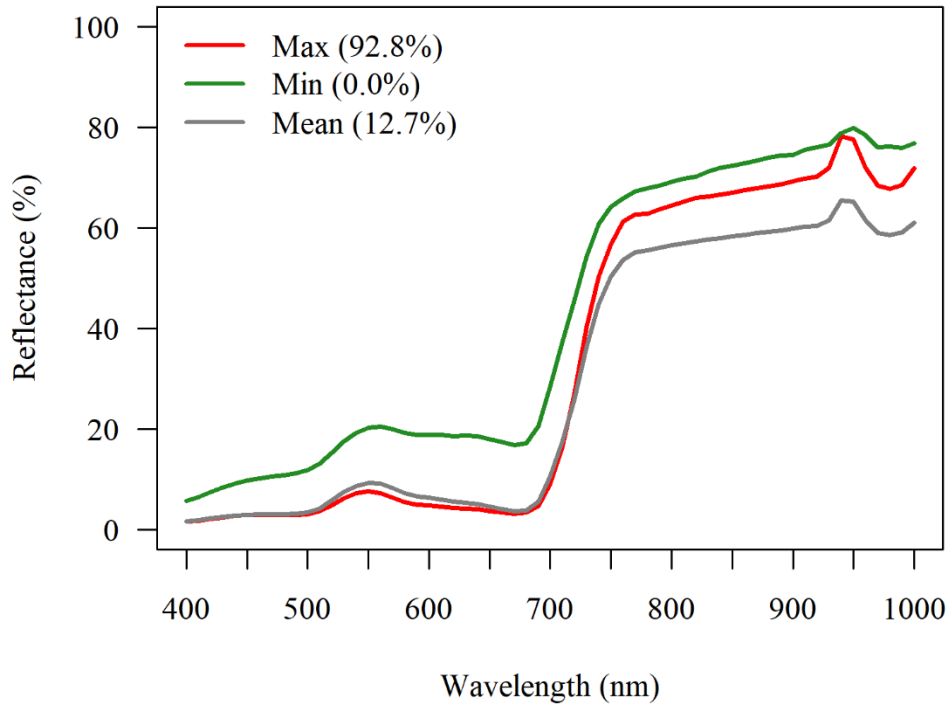
Difference spectra measurements / lab analysis ~ 3 days

Match the spectra with reference method

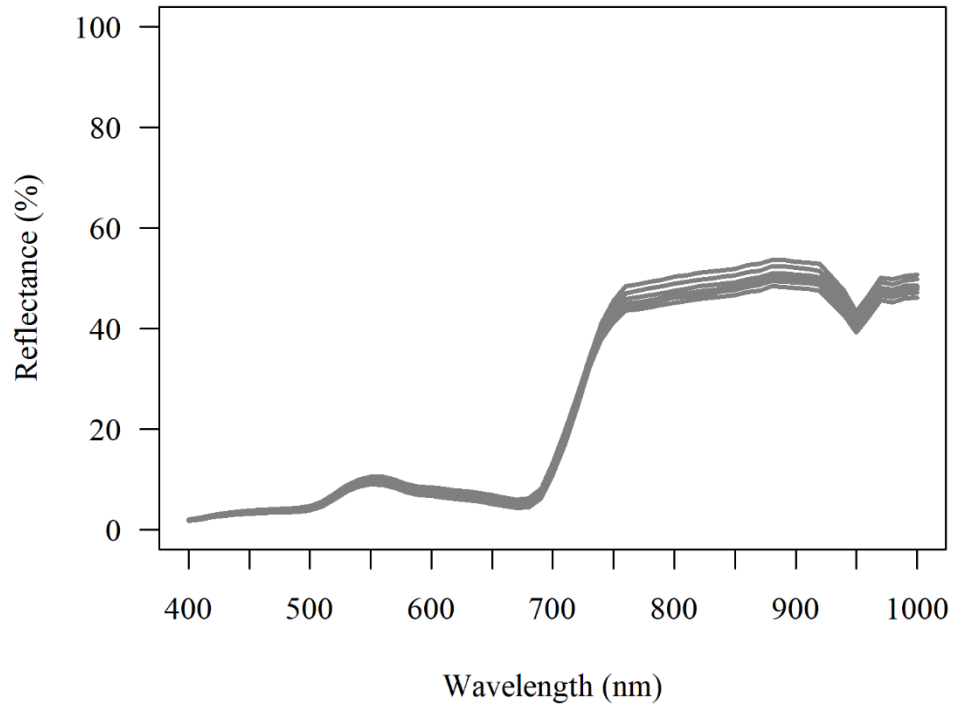
Spectra check

Difference spectra measurements / lab analysis ~ 3 days

Spectra characteristics of clover content



Spectra issues 2017 - Place 3



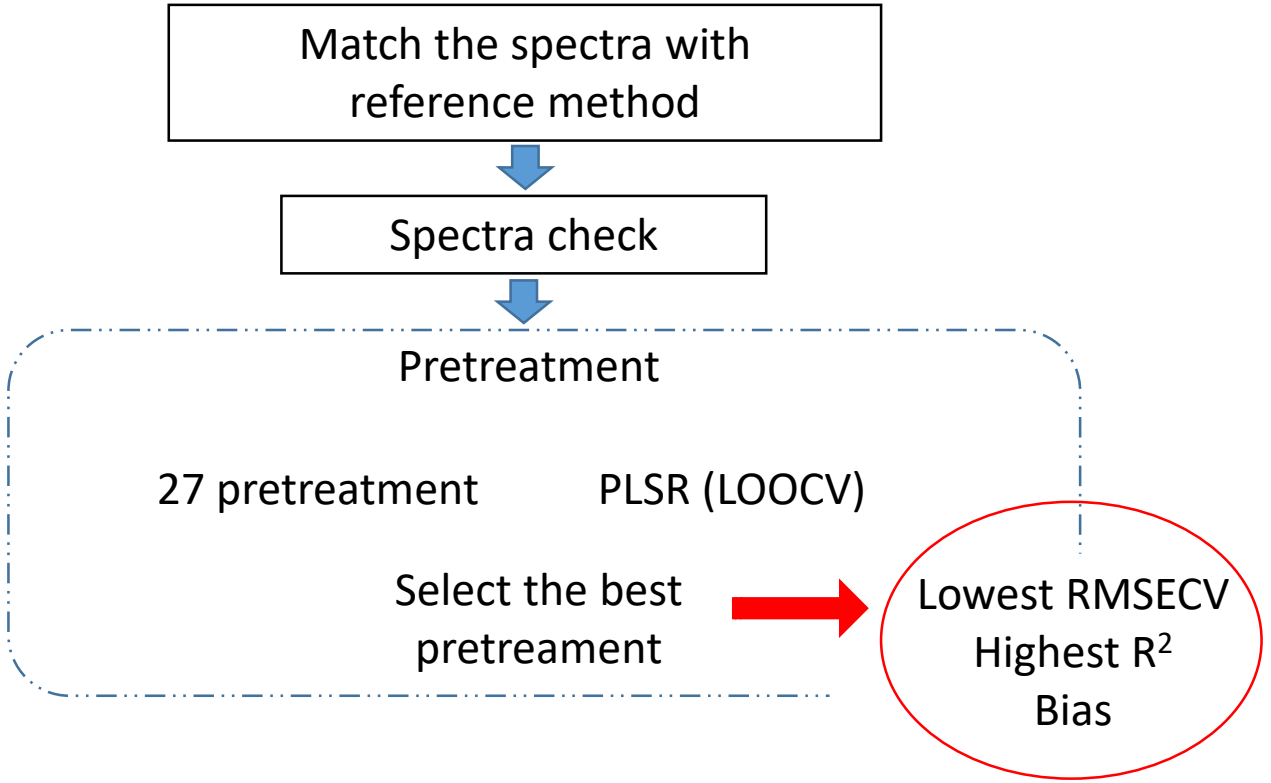
Match the spectra with reference method

Spectra check

Samples

	2017	2018	2019
CUT_1	18	71	69
CUT_2	54	54	107
CUT_3	18	36	18
klipp	36	45	48

574 samples



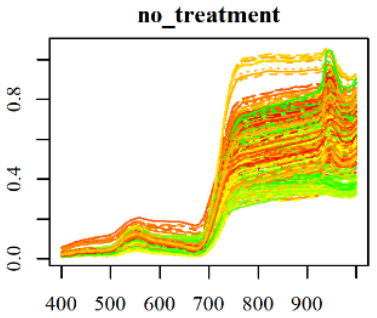
- 27 combinations (SNV, 1st derivative, 2nd derivative, MSC, mean center)

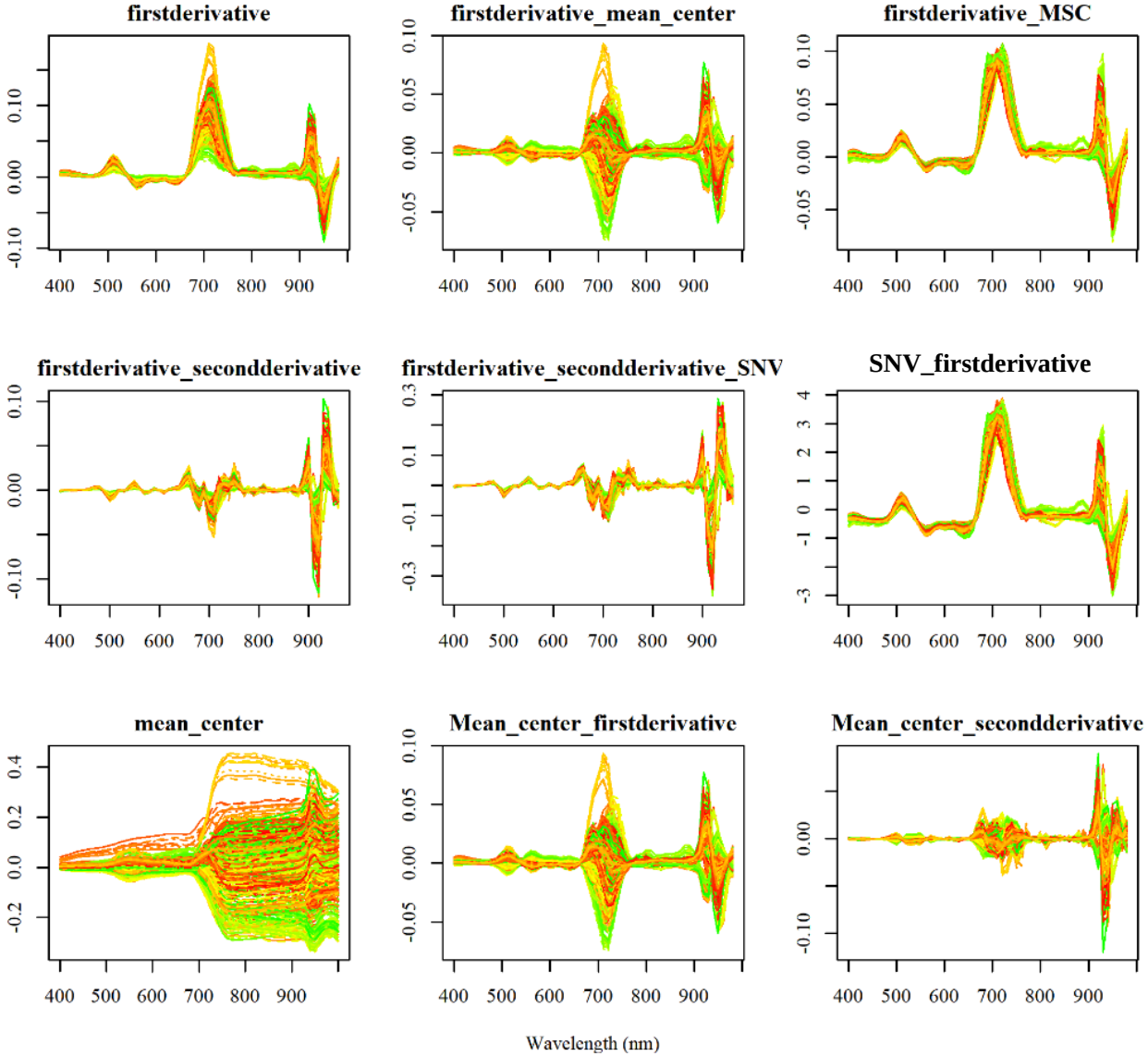
- PLS regression (standard multivariate method)

Pretreatment	R2	RMSECV	Bias
sqrt_SNV_mean_center	0.44	13.01	-1.31
SNV_mean_center	0.55	10.30	0.11
sqrt_secondderivative_firstderivative	0.66	9.26	-1.14
sqrt_firstderivative_secondderivative	0.66	9.26	-1.14
SNV_secondderivative_firstderivative	0.66	8.82	0.02
SNV_firstderivative_secondderivative	0.66	8.82	0.02
sqrt_SNV_firstderivative_secondderivative	0.66	9.00	-1.31
sqrt_SNV_secondderivative_firstderivative	0.66	9.00	-1.31
sqrt_Mean_center_secondderivative	0.67	9.09	-1.08
sqrt_secondderivative	0.67	9.09	-1.08
sqrt_secondderivative_mean_center	0.67	9.09	-1.08
sqrt_mean_center	0.68	8.85	-1.06
sqrt_no_treatment	**0.68**	**8.85**	**-1.06**
secondderivative_MSC	0.69	8.45	0.01
sqrt_secondderivative_MSC	0.70	8.47	-1.17
secondderivative_SNV	0.70	8.31	0.01
firstderivative_secondderivative	0.70	8.27	0.03
secondderivative_firstderivative	0.70	8.27	0.03
sqrt_secondderivative_SNV	0.71	8.37	-1.20
sqrt_firstderivative_MSC	0.71	8.36	-1.19
firstderivative_MSC	0.71	8.18	0.01
sqrt_Mean_center_firstderivative	0.71	8.50	-1.03
sqrt_firstderivative_mean_center	0.71	8.50	-1.03
sqrt_firstderivative	**0.71**	**8.50**	**-1.03**
secondderivative_firstderivative_SNV	0.71	8.16	0.01
firstderivative_secondderivative_SNV	0.71	8.16	0.01
sqrt_firstderivative_SNV	0.71	8.24	-1.18
firstderivative_SNV	0.72	8.09	0.01
no_treatment	**0.72**	**8.09**	**0.04**
mean_center	0.72	8.09	0.04
Mean_center_secondderivative	0.72	8.08	0.03
secondderivative_mean_center	0.72	8.08	0.03
secondderivative	0.72	8.08	0.03
MSC_secondderivative	0.72	8.00	0.01
SNV_secondderivative	0.72	8.00	0.01
sqrt_firstderivative_secondderivative_SNV	0.72	8.12	-1.14
sqrt_secondderivative_firstderivative_SNV	0.72	8.12	-1.14
MSC_mean_center	0.72	7.98	0.01
MSC	0.72	7.98	0.01
SNV	0.72	7.96	0.01
Mean_center_SNV	0.72	7.96	0.01
sqrt_SNV_secondderivative	0.73	8.07	-1.13
sqrt_MSC_secondderivative	0.73	8.06	-1.13
MSC_firstderivative	0.73	7.88	0.01
sqrt_MSC	0.73	7.97	-1.12
sqrt_MSC_mean_center	0.73	7.97	-1.12
sqrt_Mean_center_SNV	0.73	7.99	-1.12
sqrt_SNV	0.73	7.99	-1.12
SNV_firstderivative	**0.73**	**7.82**	**0.01**
Mean_center_firstderivative	0.74	7.76	0.03
firstderivative_mean_center	0.74	7.76	0.03
firstderivative	**0.74**	**7.76**	**0.03**
sqrt_MSC_firstderivative	0.74	7.87	-1.12
sqrt_SNV_firstderivative	**0.75**	**7.70**	**-1.09**

Lowest RMSECV
Highest R^2
Bias

SQRT the data because were a lot of zeros





Pretreatment	R2	RMSECV	Bias
sqrt_SNV_mean_center	0.44	13.01	-1.31
SNV_mean_center	0.55	10.30	0.11
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SNV_secondderivative_firstderivative	0.66	8.82	0.02
SNV_firstderivative_secondderivative	0.66	8.82	0.02
sqrt_SNV_firstderivative_secondderivative	0.66	9.00	-1.31
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sqrt_Mean_center_secondderivative	0.67	9.09	-1.08
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sqrt_mean_center	0.68	8.85	-1.06
sqrt_no_treatment	**0.68**	**8.85**	**-1.06**
secondderivative_MSC	0.69	8.45	0.01
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secondderivative_SNV	0.70	8.31	0.01
firstderivative_secondderivative	0.70	8.27	0.03
secondderivative_firstderivative	0.70	8.27	0.03
sqrt_secondderivative_SNV	0.71	8.37	-1.20
sqrt_firstderivative_MSC	0.71	8.36	-1.19
firstderivative_MSC	0.71	8.18	0.01
sqrt_Mean_center_firstderivative	0.71	8.50	-1.03
sqrt_firstderivative_mean_center	0.71	8.50	-1.03
sqrt_firstderivative	**0.71**	**8.50**	**-1.03**
secondderivative_firstderivative_SNV	0.71	8.16	0.01
firstderivative_secondderivative_SNV	0.71	8.16	0.01
sqrt_firstderivative_SNV	0.71	8.24	-1.18
firstderivative_SNV	0.72	8.09	0.01
no_treatment	**0.72**	**8.09**	**0.04**
mean_center	0.72	8.09	0.04
Mean_center_secondderivative	0.72	8.08	0.03
secondderivative_mean_center	0.72	8.08	0.03
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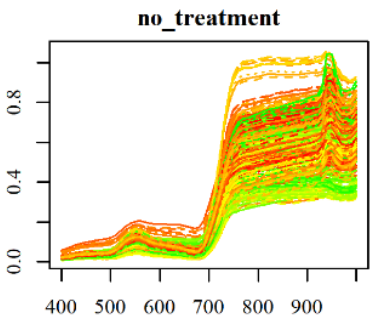
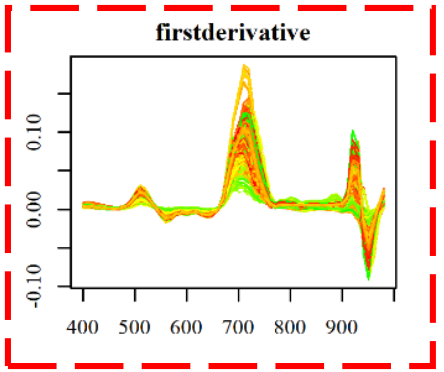
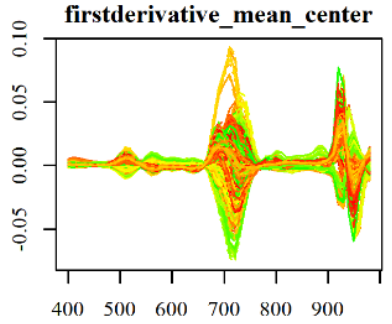
MSC_mean_center	0.72	7.98	0.01
MSC	0.72	7.98	0.01
SNV	0.72	7.96	0.01
Mean_center_SNV	0.72	7.96	0.01
sqrt_SNV_secondderivative	0.73	8.07	-1.13
sqrt_MSC_secondderivative	0.73	8.06	-1.13
MSC_firstderivative	0.73	7.88	0.01
sqrt_MSC	0.73	7.97	-1.12
sqrt_MSC_mean_center	0.73	7.97	-1.12
sqrt_Mean_center_SNV	0.73	7.99	-1.12
sqrt_SNV	0.73	7.99	-1.12
SNV_firstderivative	**0.73**	**7.82**	**0.01**
Mean_center_firstderivative	0.74	7.76	0.03
firstderivative_mean_center	0.74	7.76	0.03
firstderivative	**0.74**	**7.76**	**0.03**
sqrt_MSC_firstderivative	0.74	7.87	-1.12
sqrt_SNV_firstderivative	**0.75**	**7.70**	**-1.09**

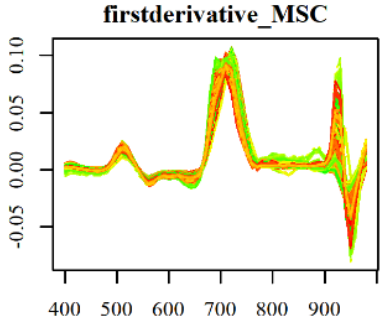
Lowest RMSECV
Highest R^2
Bias

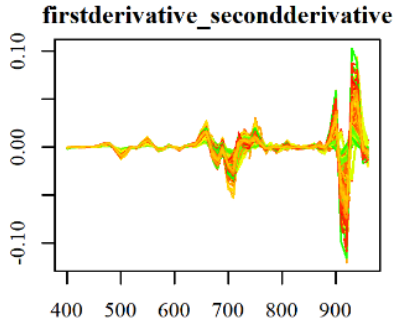
SQRT the data because were a lot of zeros

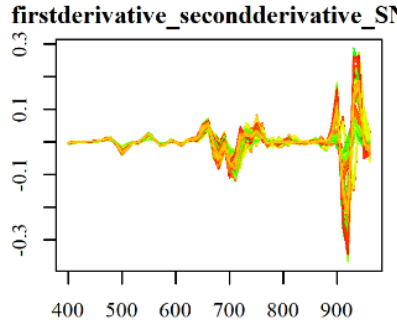


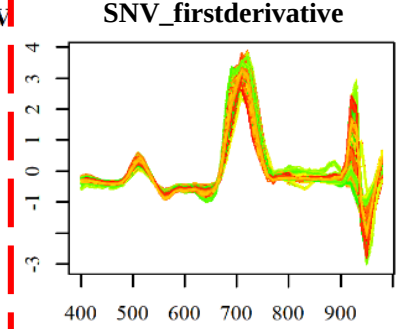


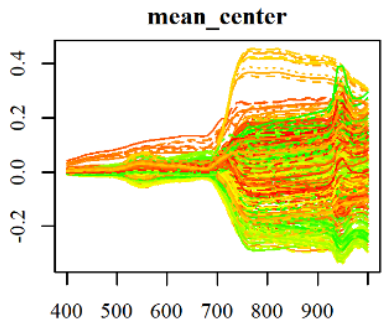


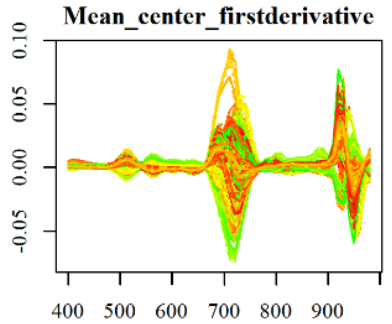


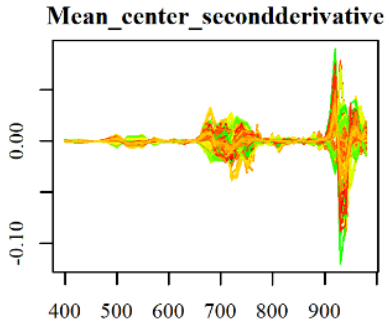




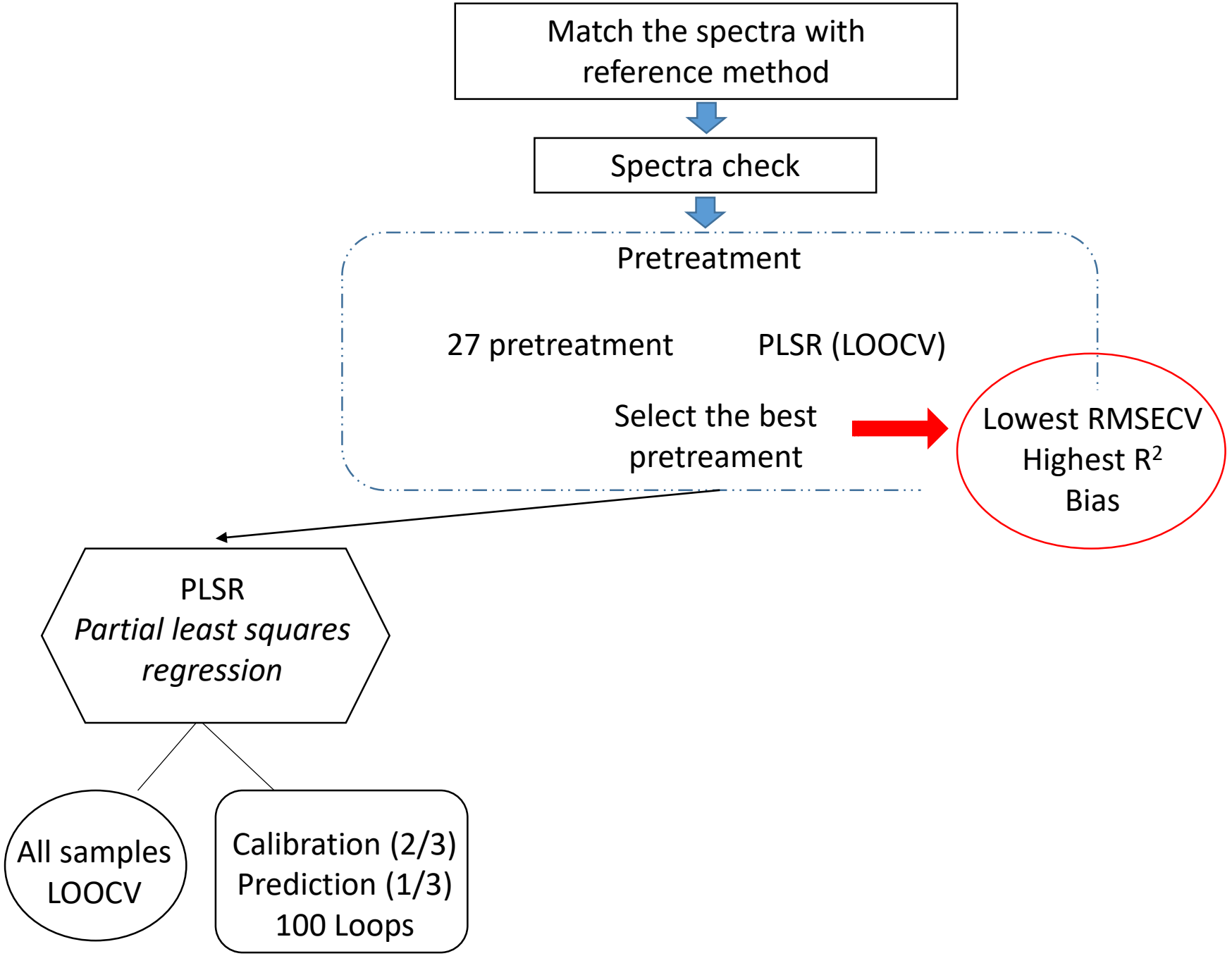


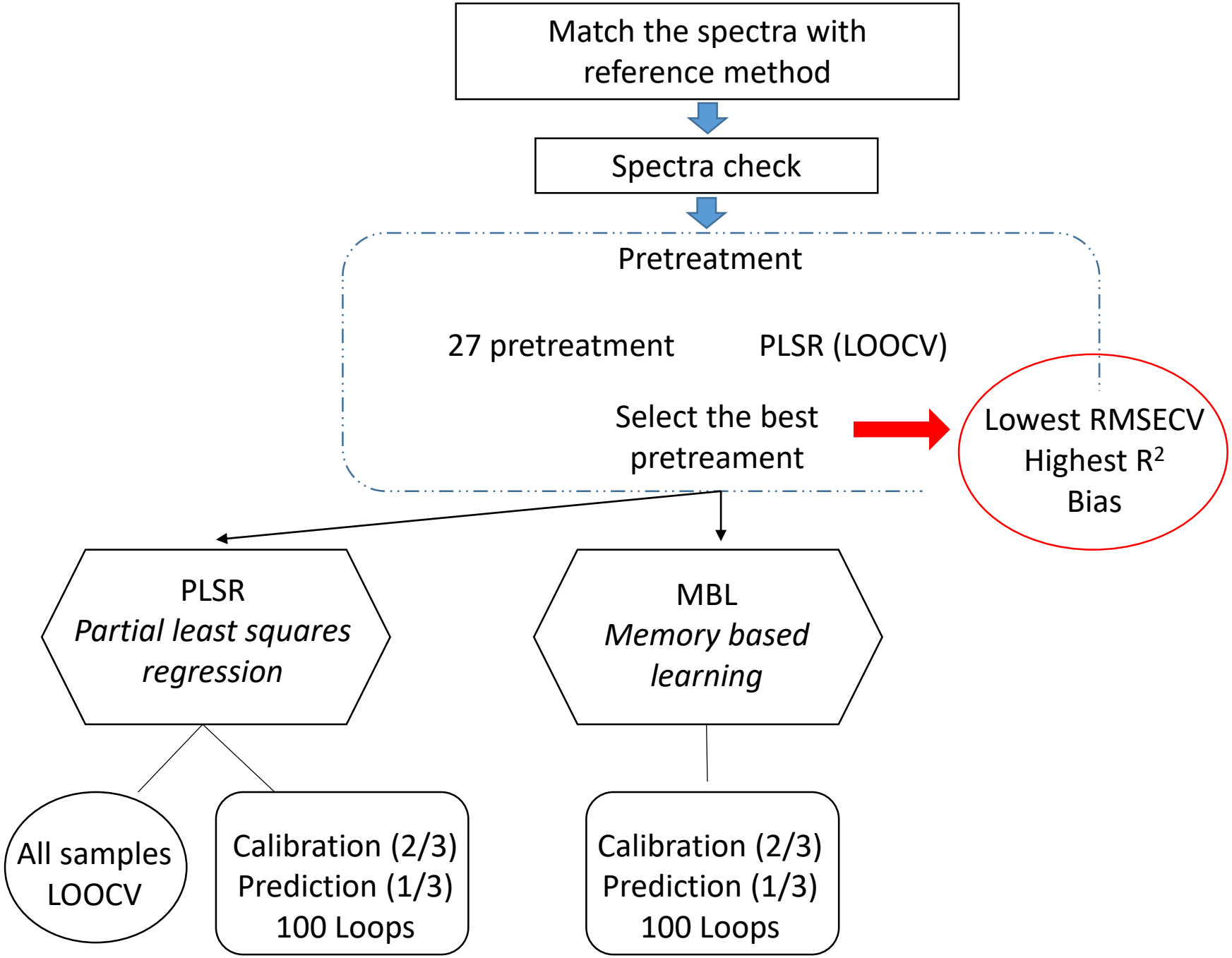






Wavelength (nm)


Match the spectra with reference method
Spectra check
Pretreatment
27 pretreatment
PLSR (LOOCV)
Select the best pretreament
Lowest RMSECV
Highest R^2
Bias
PLSR
Partial least squares regression
All samples LOOCV
Calibration (2/3)
Prediction (1/3)
100 Loops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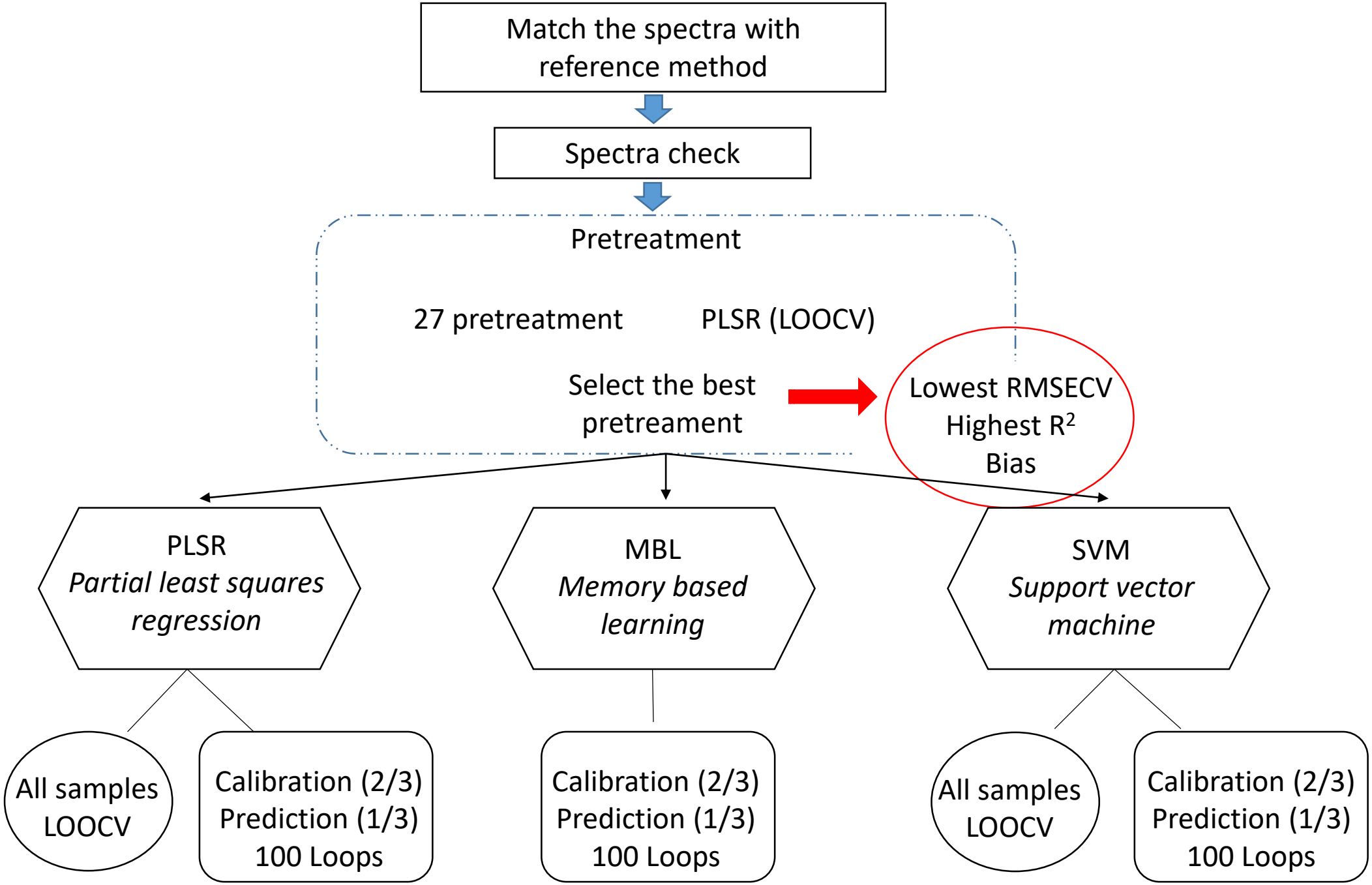
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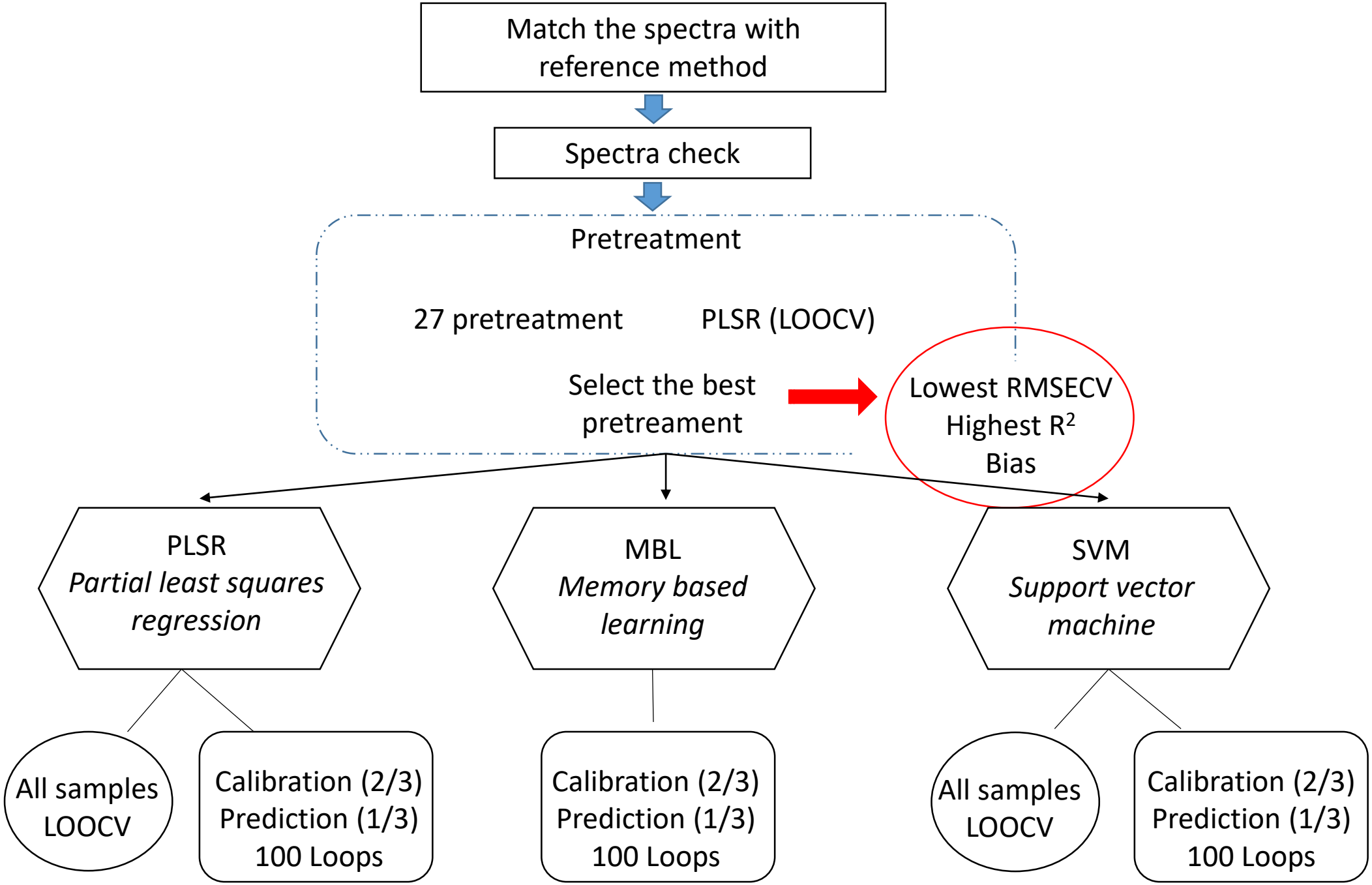
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All samples LOOCV
Calibration (2/3) Prediction (1/3) 100 Loops

Performance of multivariate models assessed

Method	samples	pretreatment	CV	RMSECV	Rsq	RMSEP	Rsq_pred
PLS	all	no_pretreatment	LOO	8.10	0.71		
		no_pretreatment_sqrt	LOO	8.90	0.68		
		1st derivative	LOO	7.76	0.74		
		1st derivative_sqrt	LOO	8.50	0.71		
		SNV_1st derivative	LOO	7.81	0.73		
		SNV_1st derivative_sqrt	LOO	7.70	0.75		
PLS	cal_val_random	no_pretreatment	LOO	8.30	0.70	8.33	0.70
		no_pretreatment_sqrt	LOO	9.11	0.67	9.31	0.66
		1st derivative	LOO	7.93	0.72	8.00	0.73
		1st derivative_sqrt	LOO	8.76	0.70	8.70	0.70
		SNV_1st derivative	LOO	8.00	0.72	8.10	0.72
		SNV_1st derivative_sqrt	LOO	7.95	0.73	7.97	0.73
MBL	cal_val_random	no_pretreatment	LNNO	7.44	0.73	7.46	0.75
		1st derivative	LNNO	7.43	0.73	7.22	0.77
		SNV_1st derivative	LNNO	7.45	0.73	7.08	0.78
SVM	all	no_pretreatment	LOO	9.66	0.62		
		no_pretreatment_sqrt	LOO	9.10	0.65		
		1st derivative	LOO	7.83	0.74		
		1st derivative_sqrt	LOO	8.30	0.71		
		SNV_1st derivative	LOO	8.18	0.71		
		SNV_1st derivative_sqrt	LOO	7.68	0.75		
SVM	cal_val_random	no_pretreatment	LOO	10.07	0.59	9.78	0.60
		no_pretreatment_sqrt	LOO	9.38	0.63	9.32	0.64
		1st derivative	LOO	8.17	0.71	7.97	0.72
		1st derivative_sqrt	LOO	8.50	0.70	8.38	0.71
		SNV_1st derivative	LOO	8.26	0.70	8.32	0.71
		SNV_1st derivative_sqrt	LOO	7.90	0.73	7.93	0.73

Performance of multivariate models assessed

Method	samples	pretreatment	CV	RMSECV	Rsq	RMSEP	Rsq_pred
PLS	all	no_pretreatment	LOO	8.10	0.71		
		no_pretreatment_sqrt	LOO	8.90	0.68		
		1st derivative	LOO	7.76	0.74		
		1st derivative_sqrt	LOO	8.50	0.71		
		SNV_1st derivative	LOO	7.81	0.73		
		SNV_1st derivative_sqrt	LOO	7.70	0.75		
PLS	cal_val_random	no_pretreatment	LOO	8.30	0.70	8.33	0.70
		no_pretreatment_sqrt	LOO	9.11	0.67	9.31	0.66
		1st derivative	LOO	7.93	0.72	8.00	0.73
		1st derivative_sqrt	LOO	8.76	0.70	8.70	0.70
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		SNV_1st derivative_sqrt	LOO	7.95	0.73	7.97	0.73
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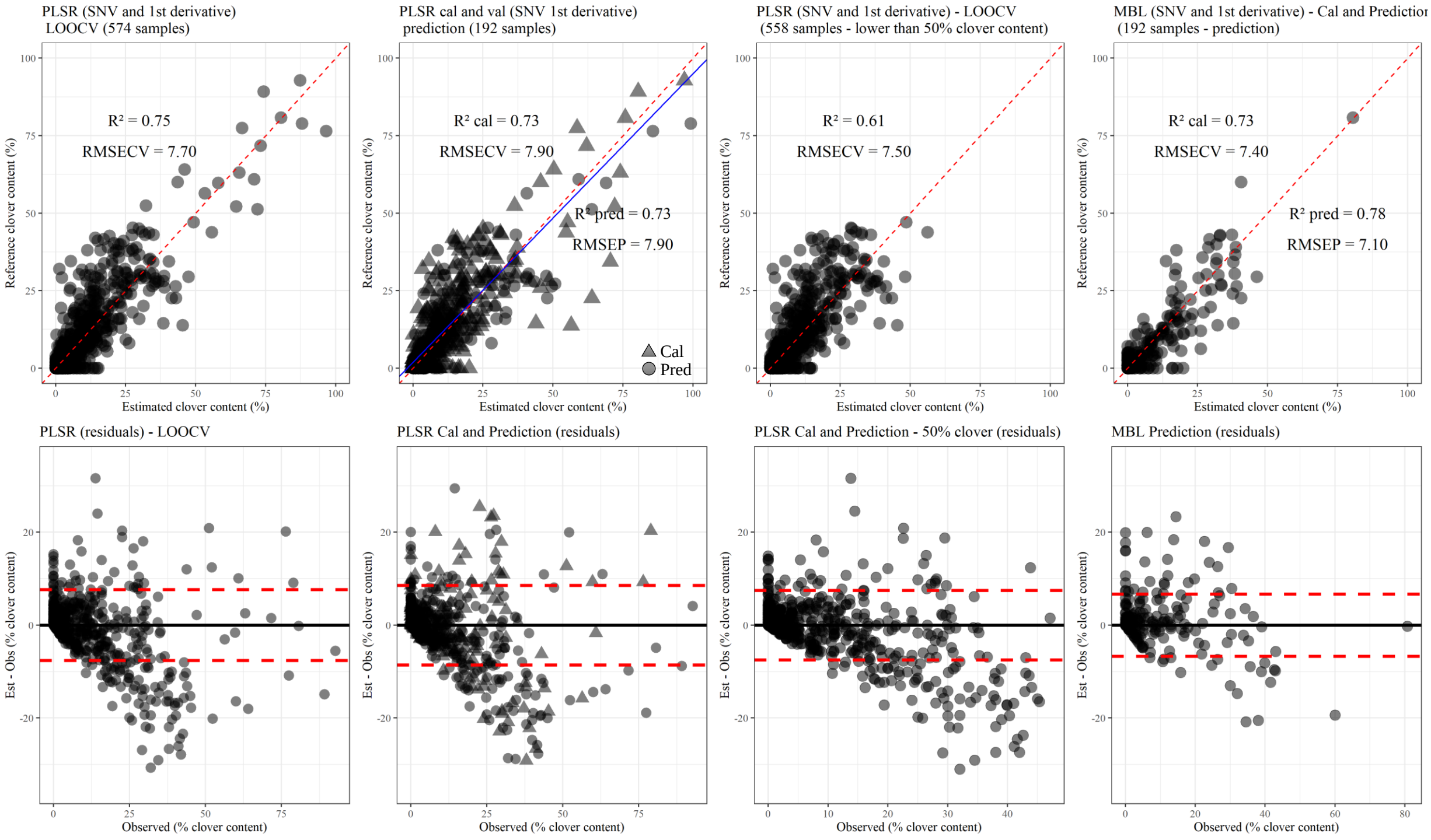
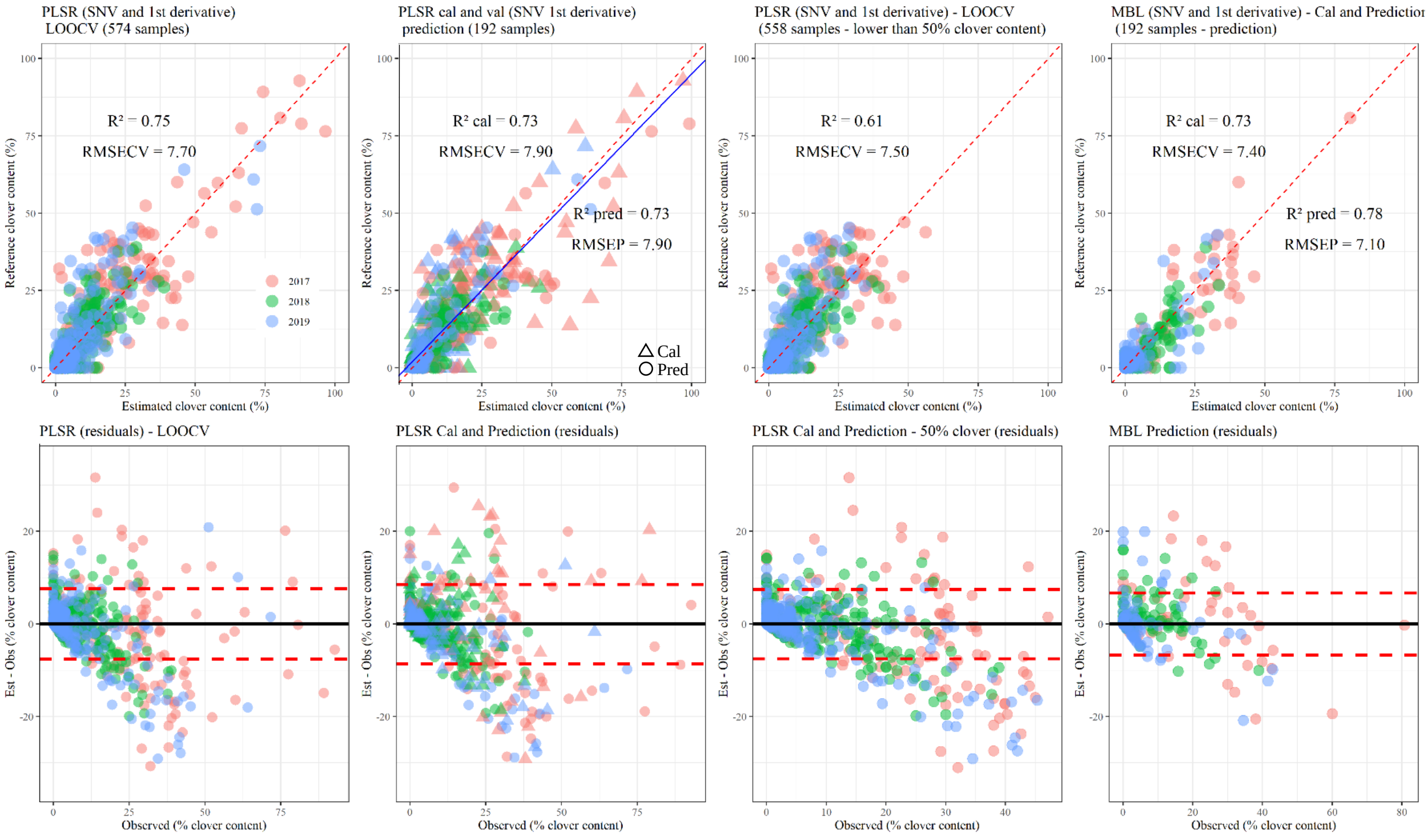

PLSR (SNV and 1st derivative)
LOOCV (574 samples)
R² = 0.75
RMSECV = 7.70
PLSR cal and val (SNV 1st derivative)
prediction (192 samples)
R² cal = 0.73
RMSECV = 7.90
R² pred = 0.73
RMSEP = 7.90
Cal
Pred
PLSR (SNV and 1st derivative) - LOOCV
(558 samples - lower than 50% clover content)
R² = 0.61
RMSECV = 7.50
MBL (SNV and 1st derivative) - Cal and Prediction
(192 samples - prediction)
R² cal = 0.73
RMSECV = 7.40
R² pred = 0.78
RMSEP = 7.10
Reference clover content (%)
Estimated clover content (%)
PLSR (residuals) - LOOCV
PLSR Cal and Prediction (residuals)
PLSR Cal and Prediction - 50% clover (residuals)
MBL Prediction (residuals)
Est - Obs (% clover content)
Observed (% clover content)


PLSR (SNV and 1st derivative)
LOOCV (574 samples)
R² = 0.75
RMSECV = 7.70
2017
2018
2019
Reference clover content (%)
Estimated clover content (%)
PLSR cal and val (SNV 1st derivative)
prediction (192 samples)
R² cal = 0.73
RMSECV = 7.90
R² pred = 0.73
RMSEP = 7.90
Cal
Pred
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(558 samples - lower than 50% clover content)
R² = 0.61
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MBL (SNV and 1st derivative) - Cal and Prediction
(192 samples - prediction)
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PLSR Cal and Prediction (residuals)
PLSR Cal and Prediction - 50% clover (residuals)
MBL Prediction (residuals)
Est - Obs (% clover content)
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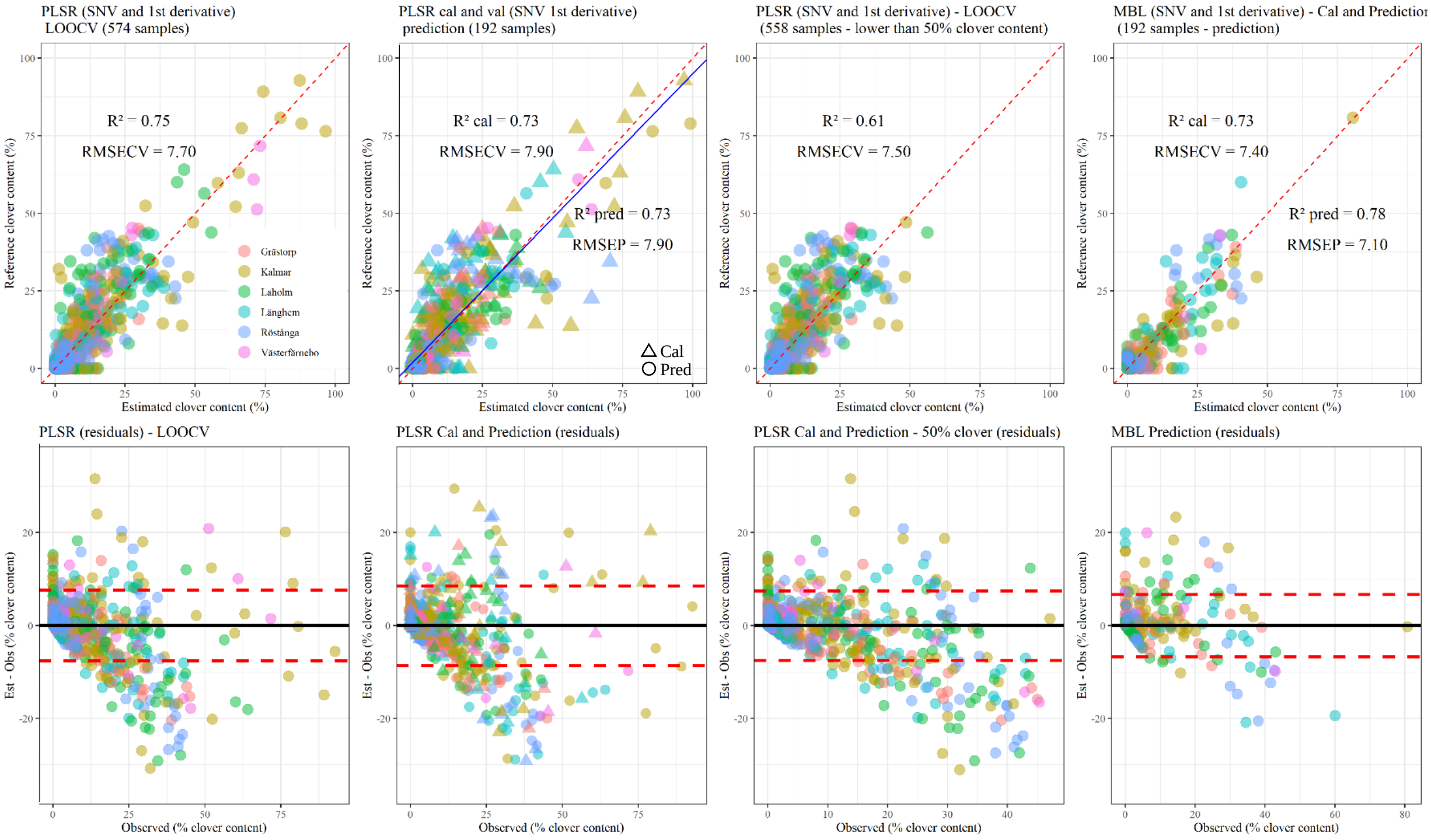
PLSR (SNV and 1st derivative)
LOOCV (574 samples)
R² = 0.75
RMSECV = 7.70
Grästorp
Kalmar
Laholm
Länghem
Röstånga
Västerfärnebo
Reference clover content (%)
Estimated clover content (%)
PLSR cal and val (SNV 1st derivative)
prediction (192 samples)
R² cal = 0.73
RMSECV = 7.90
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PLSR (residuals) - LOOCV
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PLSR Cal and Prediction - 50% clover (residuals)
MBL Prediction (residuals)
Est - Obs (% clover content)
Observed (% clover content)

Conclusions and remarks

- The YaraNSensor combined with multivariate analysis can be used with reasonable confidence to predict clover content
- Decrease the time consumption for botanical composition estimation
- Field measurements are ’tricky’ due to variation in the equipment
- Further investigation would be useful in order to improve the variability, having other datasets in different locations, for better prediction