

## Supplementary data

Tab.1 Best results from different spectral processing method for the PLS models of SH and SS contents

Parameters	Pretreated method	$PC_s$	$R_c$	$RMSEC$	$R_p$	$RMSEP$
SH ( $\mu\text{mol/g}$ )	SNV	8	0.8882	0.48	0.8392	0.61
	MSC	8	0.8884	0.49	0.8385	0.61
	1 <sup>st</sup> Der	10	0.8013	0.55	0.7855	0.78
	2 <sup>nd</sup> Der	9	0.8124	0.64	0.7756	0.74
SS ( $\mu\text{mol/g}$ )	SNV	4	0.6322	7.41	0.5814	9.66
	MSC	4	0.6312	7.45	0.5634	9.60
	1 <sup>st</sup> Der	5	0.6055	7.65	0.5044	9.89
	2 <sup>nd</sup> Der	5	0.6123	7.44	0.5146	8.78