

Supplementary Table S1. Near infrared spectroscopy pretreatment combinations used for the spectral preprocessing

Abbreviation	Pretreatment (combination)
sgol@2-13-0	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation
sgol@2-17-0	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation
sgol@2-21-0	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation
SNV	Standard Normal Variate
MSC	Multiplicative scatter correction
detr	Detrending
detr+MSC	Detrending + Multiplicative scatter correction
detr+SNV	Detrending + Standard Normal Variate
sgol@2-13-0+SNV	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Standard Normal Variate
sgol@2-17-0+SNV	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Standard Normal Variate
sgol@2-21-0+SNV	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Standard Normal Variate
sgol@2-13-0 +MSC	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Multiplicative scatter correction
sgol@2-17-0 +MSC	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Multiplicative scatter correction
sgol@2-21-0 +MSC	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Multiplicative scatter correction
sgol@2-13-0 +detr	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending
sgol@2-17-0 +detr	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending
sgol@2-21-0 +detr	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending
sgol@2-13-0 +detr +SNV	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending + Standard Normal Variate
sgol@2-17-0 +detr +SNV	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending + Standard Normal Variate
sgol@2-21-0 +detr +SNV	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending + Standard Normal Variate
sgol@2-13-0 +detr +MSC	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending + Multiplicative scatter correction
sgol@2-17-0 +detr +MSC	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending + Multiplicative scatter correction
sgol@2-21-0 +detr +MSC	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending + Multiplicative scatter correction
sgol@2-21-0 +sgol@2-21-1	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial 1 <sup>st</sup> derivative
sgol@2-21-0 +sgol@2-21-2	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial 2 <sup>nd</sup> derivative
sgol@2-21-0 +sgol@2-13-1	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial 1 <sup>st</sup> derivative
sgol@2-21-0 +sgol@2-13-2	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial 2 <sup>nd</sup> derivative
sgol@2-21-0 +sgol@2-17-1	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial 1 <sup>st</sup> derivative
sgol@2-21-0 +sgol@2-17-2	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial 2 <sup>nd</sup> derivative

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sgol@2-13-0 +sgol@2-21-2	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial 2 <sup>nd</sup> derivative
sgol@2-13-0 +sgol@2-13-1	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial 1 <sup>st</sup> derivative
sgol@2-13-0 +sgol@2-13-2	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial 2 <sup>nd</sup> derivative
sgol@2-13-0 +sgol@2-17-1	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial 1 <sup>st</sup> derivative
sgol@2-13-0 +sgol@2-17-2	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial 2 <sup>nd</sup> derivative
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sgol@2-17-0 +sgol@2-17-1	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial 1 <sup>st</sup> derivative
sgol@2-17-0 +sgol@2-17-2	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial 2 <sup>nd</sup> derivative
sgol@2-17-0 +sgol@2-13-1	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial 1 <sup>st</sup> derivative
sgol@2-17-0 +sgol@2-13-2	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial 2 <sup>nd</sup> derivative