

**Table S6 - Pretreatments of the NIR spectra**

Number	Pretreatment (combination)
1	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation
2	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation
3	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation
4	Standard Normal Variate
5	Multiplicative scatter correction
6	Detrending
7	Detrending + Multiplicative scatter correction
8	Detrending + Standard Normal Variate
9	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Standard Normal Variate
10	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Standard Normal Variate
11	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Standard Normal Variate
12	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Multiplicative scatter correction
13	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Multiplicative scatter correction
14	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Multiplicative scatter correction
15	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending
16	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending
17	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending
18	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending + Standard Normal Variate
19	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending + Standard Normal Variate
20	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending + Standard Normal Variate
21	Savitzky-Golay Smoothing 13 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending + Multiplicative scatter correction
22	Savitzky-Golay Smoothing 17 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending + Multiplicative scatter correction
23	Savitzky-Golay Smoothing 21 sample points, 2 <sup>nd</sup> polynomial no derivation + Detrending + Multiplicative scatter correction
24	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
25	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
26	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

Number	Pretreatment (combination)
27	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
28	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
29	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
30	Savitzky-Golay Smoothing 13 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
31	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
32	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
33	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
34	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
35	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
36	Savitzky-Golay Smoothing 17 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
37	Savitzky-Golay Smoothing 17 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
38	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
39	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
40	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
41	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