Pitfall in calibration developement - "chance correlation + wishful thinking" - an example of pH determination in grass silages

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The pH value of grass silages is one important parameter to determine the quality of the forages. In an attempt to use NIRS spectra taken for other quality parameter of grass silage it has been shown that a good correlation between NIR spectra of the dried forage and pH value of the fresh forage could be determined. Further investigations revealed that the B coefficients of the pH value calibration were almost the same as the B coefficients of the sugar calibration multiplied with -1. And indead the pH value - in the fresh sample material - of the calibration set is strongly correlated with the sugar concentration - in the dried sample material.

It is concluded that next to scientific tools in research the scientist and the user of NIRS equippment has to scrutinze his own work. Examples are given. NIRS is a powerfull technique, but pitfalls are present in surplus.