An evaluation of orthogonal signal correction applied to calibration transfer of near infrared spectra

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Abstract

Orthogonal signal correction (OSC) is a technique for pre-processing of, for example, NIR-spectra before they are subjected to a multivariate calibration. With OSC the **X**-matrix is corrected by a subtraction of variation that is orthogonal to the calibration **Y**-matrix. This correction can then be applied to new spectra that are going to be used in predictions. The aim of this study is to investigate if the OSC transform makes the spectra less dependent of instrument variation. This may result in easier calibration model transfer between different instruments without creating or re-analysing the whole calibration sample set. OSC was applied to NIR-spectra that were used in a calibration for the water content in a pharmaceutical product. Partial Least Squares calibrations were then compared to other calibration models with uncorrected spectra, models with spectra subjected to multiplicative signal correction, and a number of other transfer methods. The performance of OSC was on the same level as for piece-wise direct standardisation and spectral offset correction for each individual instrument and PLS-models with both instruments included. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

The advantage with NIR-spectrometry includes that the measurements are non-destructive and the possibility to use solid samples without sample pretreatment. The efficient use of quantitative NIR methods is dependent on calibrations that are valid with the same instrument for an extended time. It is also of great interest if the same spectral library can be used in another location with another instrument. One single instrument also changes with time due to wear and lamp changes. In order to transfer the spectra or the calibration to a new instrument, a number of different methods exist.

A transfer method was suggested by Shenk and Westerhaus [1,2]. Here the wavelength scale is scaled by a wavelength standard, then the intensity scale is

scaled in an univariate way for each wavelength using ≈ 30 standards.

Successful transfer of calibrations has been made in the oil industry measuring octane numbers [3], by using piecewise direct standardisation (PDS) [2,4]. The efficiency of this method is based on the assumption that it is possible to characterise each instrument with fewer standards than the number needed for a full calibration or identification. The transfer standards have to be stable enough to have the same spectrum over several years to be of use in characterisation of ageing instruments. Batches of standards should be consistently produced to have the same spectrum between individual standards. This facilitates transfer of spectra since each participant in a transfer relation can have a set of standards. A recent development of PDS is the addition of a separate background correction [4]. Standards have also been used to do bias correction for MLR calibrations [5]. Transfer of calibrations without standards is shown in [6] where finite impulse response filtering is made towards an average spectrum for the target instrument. Another possibility is the use of wavelets [7].

The calibration or identification may also be developed concurrently for several instruments with additional adjustments to simulate instrumental variation. These adjustments may also be done artificially with the instrument software [8]. A review by Bouveresse and Massart [9] covers several applications involving near infrared calibration transfers.

It is also possible to add a new instrument to a calibration afterwards by keeping the previous calibration and adding spectra acquired with the new spectrometer, provided that the spectrometers are of the same type. This may be facilitated by multiplicative signal correction (MSC) [10] as indicated in a review by de Noord [11]. In this context we became interested in the possible calibration transfer benefits of orthogonal signal correction (OSC) [12]. Because OSC was not developed especially for calibration transfer it is not the objective of this paper to show that OSC is superior to other calibration transfer techniques or transformation methods. The objective is rather to investigate how OSC performs compared to other methods.

This article contains an evaluation of the possibility to use OSC to remove instrument specific features from the spectra before a calibration model is developed. OSC is operating by removing the largest features that are possible to model, without removing the information related to the analyte variation described by a Y-vector or matrix. Along with the instrument differences other variations may also be removed. Calibrations for water content in an active pharmaceutical compound were used as a test case. These were originally developed separately for two spectrometers of the same type at two laboratories. The spectrometers used different sample presentation methods.

2. Theory

The main idea in OSC is to reduce the variation in $\mathbf{X}$ not correlated to $\mathbf{y}$. In the following algorithm it is assumed that the $\mathbf{X}$ matrix, which consists of one block, X_A, for instrument A and a second block, X_B, for instrument B, and the $\mathbf{y}$ vector are centered. The $\mathbf{X}$ matrix is centered in two ways, either by using an average spectrum from the whole $\mathbf{X}$ matrix (global centering), or by using one average spectrum for each instrument (local centering). Local centering for instrument A and B is given by

$$X_A = X_A - \bar{\mathbf{x}}_A \tag{1}$$

$$X_B = X_B - \bar{\mathbf{x}}_B \tag{2}$$

and global centering for the whole $\mathbf{X}$ matrix is given by

$$\mathbf{X} = X - \bar{\mathbf{x}} = \begin{bmatrix} X_A \\ X_B \end{bmatrix} - \frac{N_A \bar{\mathbf{x}}_A + N_B \bar{\mathbf{x}}_B}{N_A + N_B} \tag{3}$$

where N_A and N_B are the number of spectra in X_A and X_B respectively. The $\mathbf{y}$ vector is always globally centered because the reference measurement is not related to the instrument differences.

2.1. Algorithm

The first step in the algorithm is to calculate one score vector t using PCA. This vector is centered

$$t = t - \bar{t} \tag{4}$$

and then orthogonalized to y (already centered)

$$t_\perp = t - \frac{y't}{y'y} y. \tag{5}$$

Then add the average t

$$t^* = t_\perp + \bar{t}. \tag{6}$$

This vector is now orthogonal to y.

Next, calculate a loading vector w by

$$w = t^{*'}X/(t^{*'}t^*) \tag{7}$$

and scale to the unit length

$$w = w/\sqrt{w'w} \tag{8}$$

Now calculate a new t vector

$$t = Xw. \tag{9}$$

Repeat Eqs. (4)–(9) until t^* becomes stable.

The final t^* is now a good descriptor of the part of X that is orthogonal to y. Other ways to calculate an orthogonal t^* are discussed further by Wold et al. in this issue [12].

The next step in the OSC-algorithm is to make a PLS model with X calibrated against t^*. Here we use many PLS-components to ensure that t^* is well described by the model, thus approaching a MLR model. We need more components than usual in the prediction of t^*, since the aim is to model the part of the non-random variations that are smaller than the dominating y-variations. A part of these variations is due to the instrument differences. To achieve this, up to 15 components were used in this work.

Calculate the prediction vector $\hat{b}$:

$$w^{*'} = \hat{b} = \mathbf{W}(\mathbf{P}'\mathbf{W})^{-1}\hat{q} \tag{10}$$

where $\mathbf{W}$ is a matrix containing the 15 weight vectors from the PLS model above, $\mathbf{P}$ is a matrix con-
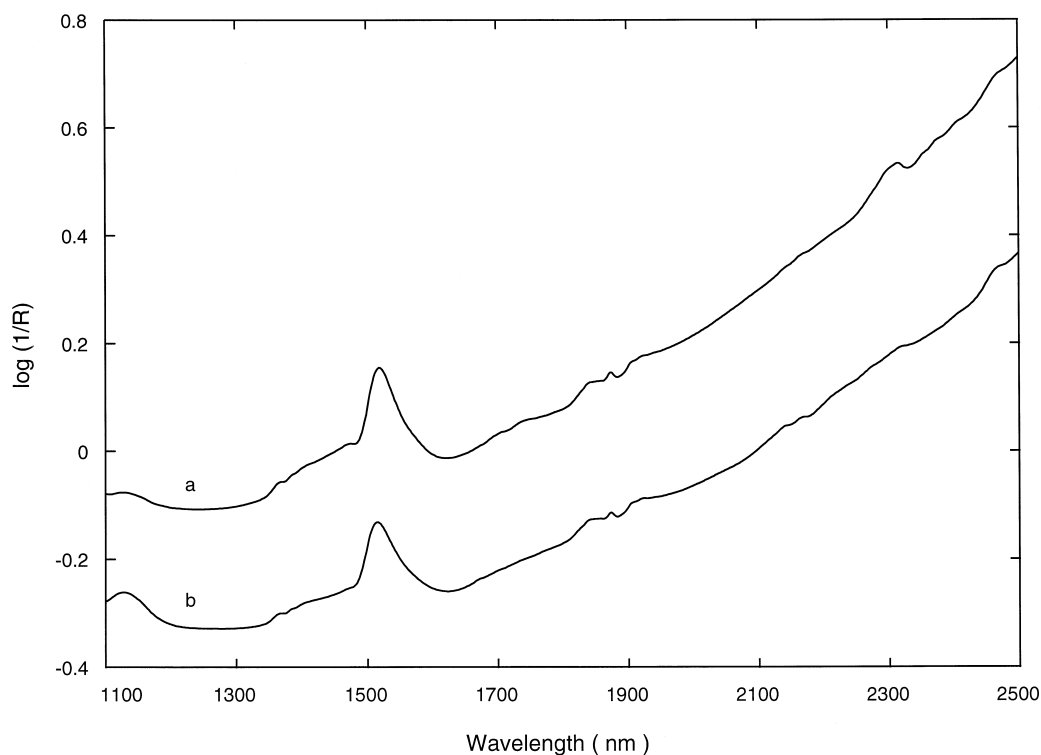

Fig. 1. Spectra of the internal ceramic reference plates. The Wood's anomaly is visible as a peak at ≈ 1500 nm and a similar feature is present at 1150 nm. (a) Instrument A, (b) instrument B.

taining the corresponding 15 loading vectors and $\hat{\boldsymbol{q}}$ is a vector containing the 15 regression coefficients for the inner relation between $\boldsymbol{t}^*$ and each score vector in the 15 component PLS done above.

Then calculate $\boldsymbol{t}^{**}$

$$\boldsymbol{t}^{**} = \boldsymbol{X}\boldsymbol{w}^*. \tag{11}$$

Calculate an $\boldsymbol{X}$-loading vector

$$\boldsymbol{p} = \boldsymbol{X}'\boldsymbol{t}^{**}/(\boldsymbol{t}^{**}{}'\boldsymbol{t}^{**}) \tag{12}$$

and subtract the information orthogonal to the original $\boldsymbol{y}$:

$$\boldsymbol{X}_{\text{OSC}} = \boldsymbol{X} - \boldsymbol{t}^{**}\boldsymbol{p}' \tag{13}$$

Several OSC-components can be removed by repeating the steps above. As $\boldsymbol{w}^*$ is a summary of all the PLS components in the local model, we do not reduce the dimension or rank of the data with more than one per OSC-component.

2.2. Correction of new spectra

To make a correction of new spectra, first center with the appropriate average spectrum calculated in the first transformation. Then calculate a score $\boldsymbol{t}$

$$\boldsymbol{t} = \boldsymbol{x}\boldsymbol{w}^* \tag{14}$$

and then remove the OSC-component by using the loading $\boldsymbol{p}$

$$\boldsymbol{X}_{\text{OSC}} = \boldsymbol{X} - \boldsymbol{t}\boldsymbol{p}'. \tag{15}$$

If several OSC-components are to be removed, repeat from Eq. (14).

When taking away information not correlated to $\boldsymbol{y}$ we have to assume that $\boldsymbol{y}$ has no noise (which is not always the case). This means that some variation in $\boldsymbol{X}$ correlated to the true $\boldsymbol{y}$ may be removed. This is however always the case in multivariate calibration and just brings back the problem to accurate reference-measurements.

2.3. Diagnostic tools

In this study we used two different ways to select the number of OSC components. First we observed that scores for the different instruments remained grouped if only one OSC component was removed. After removing a second OSC-component, the instrument variation was no longer visible in the score plots. The second approach was to calculate the removed variance of $\boldsymbol{X}$ after each OSC component i.

$$R_i^2 = \frac{\text{var}(\boldsymbol{X}_i)}{\text{var}(\boldsymbol{X})} \tag{16}$$

This value will reach a certain level after a number of OSC components. A condition for convergence of

Table 1
Summary of the calibration models used in transfer test 1–3

Model name	Signal correction method[a]	Spectral centering	PLS-components[b] in calibration for instrument A	PLS-components[b] in calibration for instruments A + B
UC 1	Uncorrected	none	4	4
UC 2	Uncorrected	local	4	4
MSC	Multiplicative signal correction	none	4	4
SNV	Standard normal variate	none	4	4
Der	2nd derivative	none	3	3
WLS	Removed wavelengths[c]	none	4	4
PDS	Piecewise direct standardisation[d]	none	4	4
Der + OSC	2nd derivative + OSC (1 component)	none, global	2	3
SNV + PDS	SNV + PDS	none	4	3
OSC 1	OSC (2 components)	global	2	2
OSC 2	OSC (2 components)	local	2	2

[a] All spectra from instrument A and B in data set 1 where used in the signal correction.
[b] Cross validation statistics were used to determine the number of components.
[c] 1100–1200, 1475–1600 and 2200–2500 nm were removed. Second region removed due to Wood's anomaly.
[d] Piecewise direct standardisation with additive background correction.

R_i is that t^{**} (Eq. (11)) is orthogonal to y. This can be calculated as $y't^{**}$ and should always be checked. These conditions were satisfied for 2 OSC components.

2.4. Measure of transfer quality

As a measure of quality of the calibration transfer, RMSEP (root mean square error of prediction) and bias was chosen,

$$\text{RMSEP}_{A-B} = \sqrt{\frac{\sum_{i=1}^{n} (y_A - y_B)^2}{n}} \qquad (17)$$

$$\text{bias}_{A-B} = \text{abs}\left(\frac{\sum_{i=1}^{n} (y_A - y_B)}{n}\right) \qquad (18)$$

where y_A denotes the predictions from instrument A and y_B denotes the predictions from instrument B.

The RMSEP is a measure of total deviation and the bias is a measure of systematic deviation [13].

3. Experimental

The data consists of NIR spectra of an active pharmaceutical compound in glass vials and their water content (in weight/weight percent) determined by Karl–Fischer titration.

3.1. Instrumental

Two NIRSystems 6500 spectrometers with DCA modules (Foss, Denmark) were used during data acquisition. All samples were contained in glass vials and diffuse reflectance spectra were obtained through the bottoms of the non-spectroscopic grade vials. Instrument A had an iris centring device (a diaphragm withdrawn during measurement) and instrument B used a stationary anodised aluminium mask to posi-
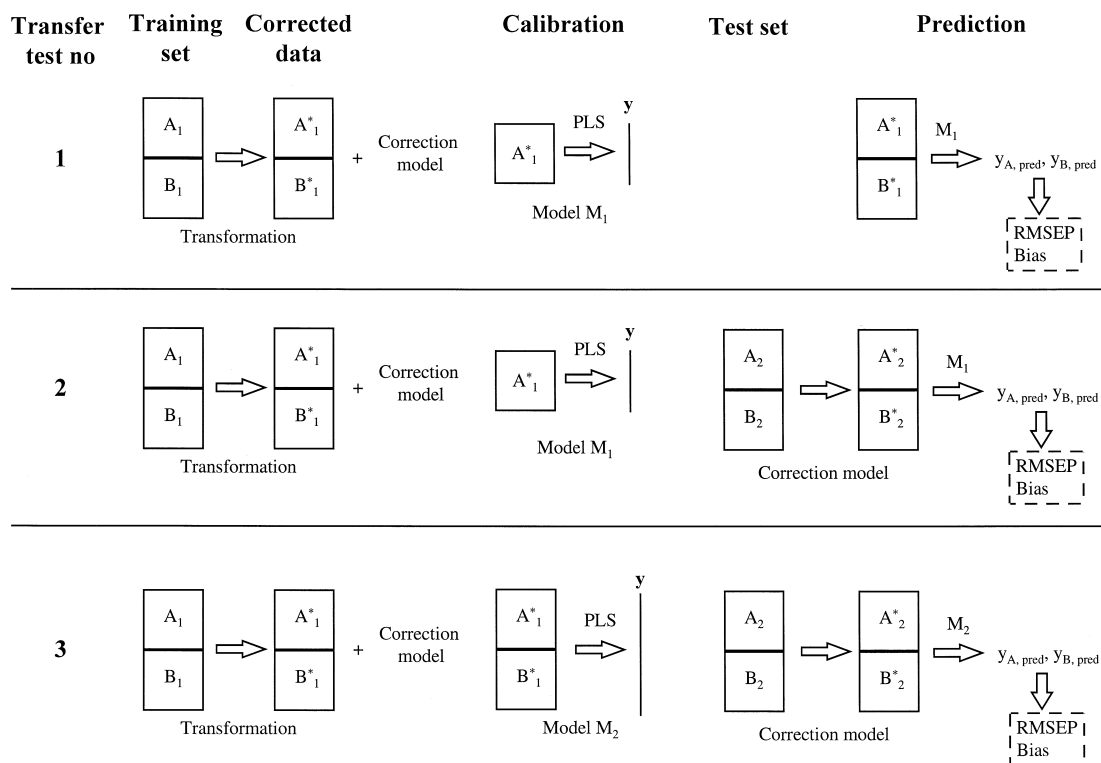

Fig. 2. Description of the different calibration transfer tests.

tion the sample. This mask was also kept in place during reference measurements. NIR spectra were measured by diffuse reflectance in the wavelength range 1100–2498 nm. The instrument ceramic reference was used as background. The spectra of the ceramic plates are shown in Fig. 1. These spectra include spectrometer differences and are used to correct the spectra to zero base line.

3.2. Software

Vision 1.00, and NSAS 3.27 (Foss, Denmark) were used for data acquisition for instruments A and B respectively. The OSC, standard normal variate (SNV), local centering and PDS calculations were performed in MATLAB 4.2c (MathWorks, Natick, USA). The PLS_Toolbox Version 1.5.2 (Eigenvector Technologies, Manson, USA) was used for the PDS calculations. MSC, second derivative, wavelength se-

lection and all the PLS calibrations were made in The Unscrambler 6.11a (CAMO, Trondheim, Norway). All the programs were run on an IBM compatible PC.

3.3. Data set 1

Data set 1 consists of spectra from 15 batches specially selected to cover a variation of the water content. The spectra were first collected on instrument B (50 scans/spectrum) and then three days later, measured on instrument A (32 scans/spectrum). Two spectra were measured for each batch on each instrument ($15 \times 2 \times 2 = 60$ spectra). The second measurement was done after a 90° rotation of the glass vial. A reference spectrum was measured every second spectrum to avoid drift in the spectrometer. The vials were kept tightly closed with lids until the final reference measurement. After the last NIR measurement the reference values for the water content
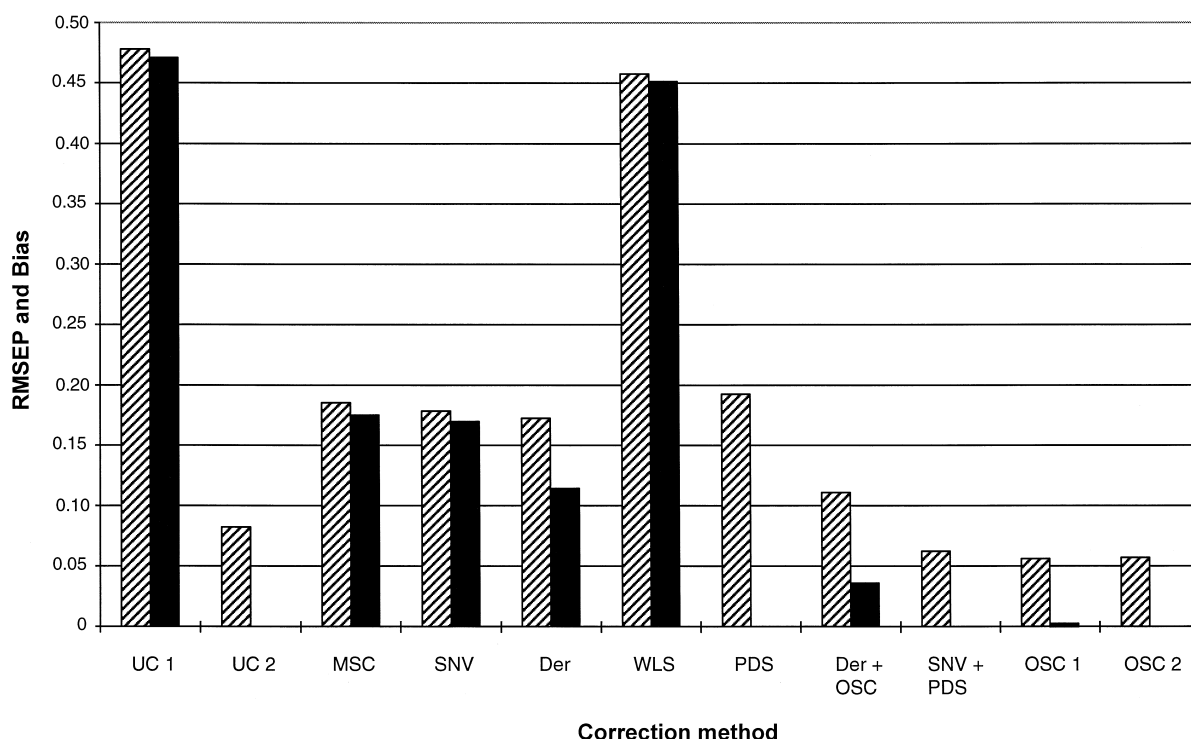

Fig. 3. RMSEP and bias (striped and black bars) for different correction methods (according to Table 1). Models on instrument A (data set 1). Predictions for instruments A and B (data set 1). Bars for the bias are too small to be seen on this scale for UC2, PDS, SNV + PDS, and OSC 2.
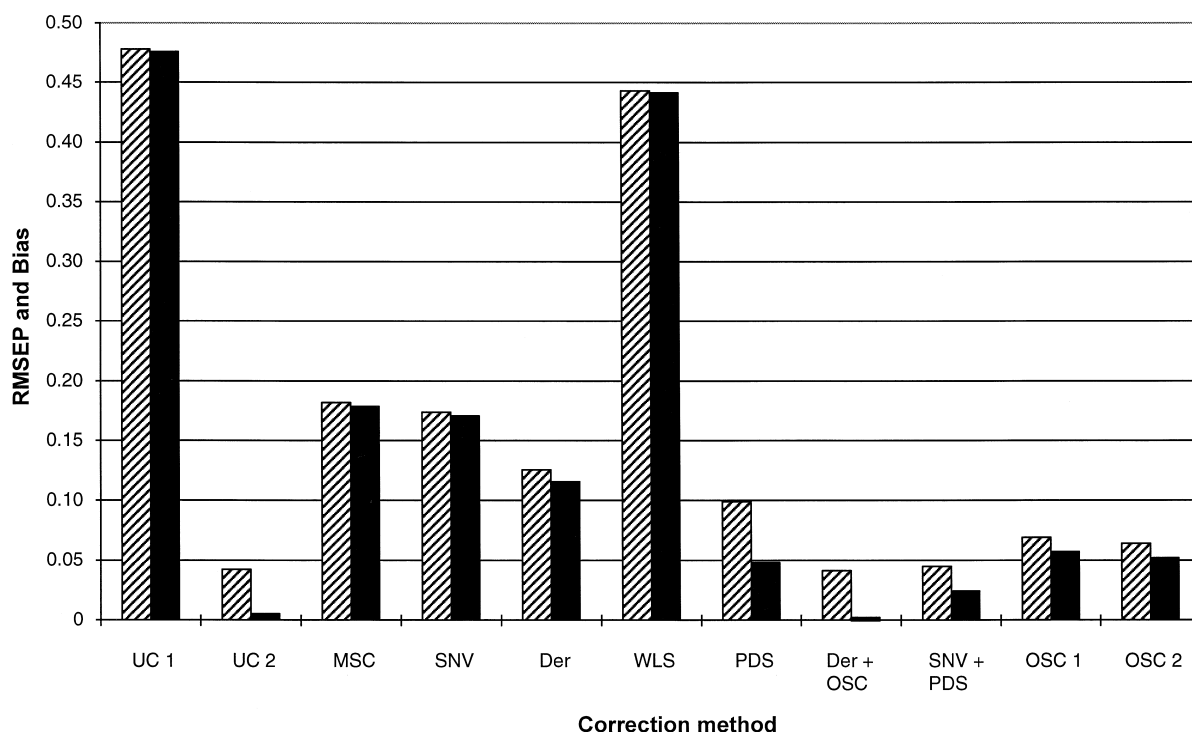
Fig. 4. RMSEP and bias (striped and black bars) for different correction methods (according to Table 1). Models on instrument A (data set 1). Predictions for instruments A and B (data set 2). The bias bars for Der + OSC and UC 2 may be too small to be seen on this scale.

were determined by Karl–Fischer titration. The reference values varied from 1.38 to 4.47 wt./wt.%.

3.4. Data set 2

Data set 2 contains 100 spectra from 5 selected batches. There were 5 vials from each batch and each vial was measured twice with a vial rotation of 90° between the measurements. Spectra were first measured on instrument A and 2 days later spectra were measured on instrument B. During the whole procedure the vials were kept tightly closed. A reference spectrum was measured for every 10th spectrum. For both instruments 32 scans per spectrum were used. Karl–Fischer titration was not performed on the samples in data set 2. Estimated values for the water content in data set 2 were 1.4–3.2 wt./wt.%.

3.5. Data transformations

In order to compare the OSC to other signal correction techniques a number of transformations were made before making the calibrations. The first (UC-1) was based on uncorrected spectra without centering before the calibration, and the second transformation (UC-2) was based on locally centered spectra. The instrumental averages were stored for future predictions.

MSC [10] and SNV [14] transformation were used as transformation methods 3 and 4. The fifth transformation (Der) was based on second derivative spectra. The derivation was done using a length 5 Savitzky–Golay filter. These three spectral pre-treatment methods are commonly used in multivariate calibrations.

Wavelength selection (WLS) was done by removing wavelength regions with known instrumental variations. The rationale for removing the wavelength regions 1100–1200, 1475–1600 and 2200–2500 was that in the first region a known instrumental artefact is present and in the second region the Wood's anomaly [15] occurs. The third region has lesser dynamic range.

In transformation 6 PDS with additive background correction [2] was used to transfer spectra from instrument B to instrument A spectra. No centering was done prior to the standardisation.

Transformation 7, (Der + OSC) was a combination of second derivative spectra followed by globally centered OSC correction (1 OSC component). In transformation 8, (SNV + PDS) spectra were first transformed with SNV, then converted by PDS.

The last two transformations were two OSC transformations where 2 OSC-components were removed. The difference was that in the OSC 1 transformation global centering was used and in OSC 2 local centering was used.

Spectra used in the calibration set were always centered before calibration, but after the transformations. The number of PLS components was determined by cross-validation and RMSEP. In Table 1, the model names, transformations, type of centering and numbers of PLS-components are summarised.

3.5.1. Calibration transfer test 1

Data transformations were performed using all spectra from instrument A and B in data set 1 (A_1 and B_1). The calibrations were then made on spectra from instrument A only. Predictions were made for all spectra from instrument A and B in data set 1.

3.5.2. Calibration transfer test 2

Data transformations were done using all spectra in data set 1. The calibrations were then performed on spectra from instrument A in data set 1. All spectra in data set 2 (A_2 and B_2) were then transformed in the same way as the spectra in data set 1. The water content from both instruments in data set 2 was predicted.

3.5.3. Calibration transfer test 3

Data transformations were performed using all spectra in data set 1. The calibrations were then per-
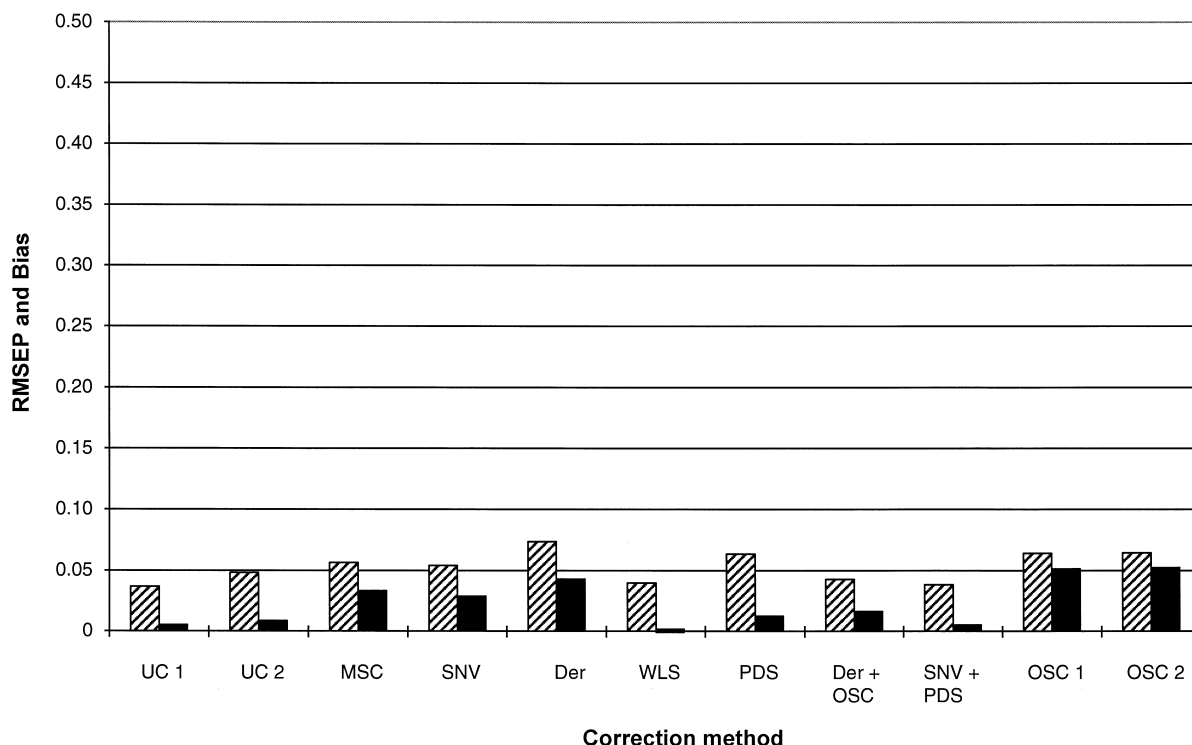

Fig. 5. RMSEP and bias (striped and black bars) for different correction methods (according to Table 1). Models on instruments A and B (data set 1). Predictions for instruments A and B (data set 2). Bias bars for UC 1, WLS and SNV + PDS may be too small to be seen on this scale.
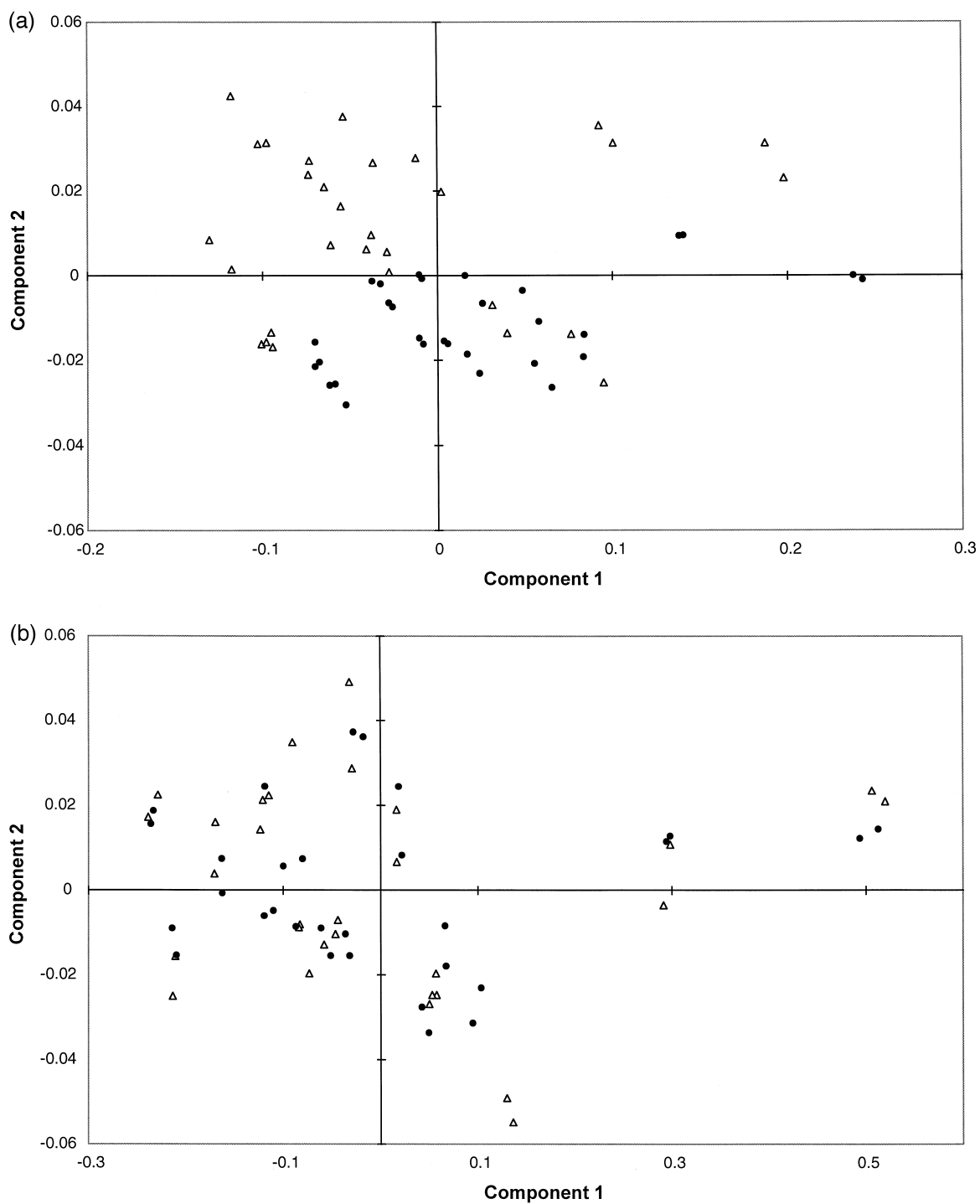
Fig. 6. Score plots for (a) MSC treated model with 85% variance in the first component and (b) OSC model with ≈ 100% variance in the first component. Triangles represent instrument A, filled circles represents instrument B.

formed on spectra from both instruments in data set 1. Predictions were then made on data set 2 (after corresponding transformation). This test was made to see how the different data transformations performed when calibrating on spectra from both instruments. All calibration transfer tests are illustrated in Fig. 2.

4. Results and discussion

The two instruments are of the same brand and same type. Hence the change of spectral response when moving to the second instrument was expected to be relatively small. In Fig. 1 we observe the differences in sampling conditions between the instruments mainly as an offset between the two ceramic plate spectra. Another visible difference in the reference spectra is the position of the peaks at 1125 and 1500 nm respectively. The peak at 1500 nm is caused by Wood's anomaly [15]. This is an unwanted polarisation effect caused by the lines of the grating. The width of this effect is slightly different between the instruments. In this case spectral translation problems are present at the peak slope on the long wavelength side.

In addition to this, the vials used to contain the samples in the spectrometer had uneven glass thickness both between vials and within the same vial. This caused baseline shifts for the individual spectra. We observed that the difference in offset between the average spectra for instrument A and B in data set 1 and 2 was not the same. This indicates that the offset is affected not only by instrument difference, but also by the sample or sample container properties.

4.1. Calibration transfer

The RMSEP and bias between predictions from the two instruments for the same samples were used in the comparison as shown in Eqs. (17) and (18). The RMSEP between the instrument responses and the Karl–Fischer titration was found to be around 0.1 wt./wt.%. The results from the calibration transfer

test 1 and 2 (only spectra from instrument A included in the calibration models) are summarised in Figs. 3 and 4. Fig. 3 contains the results when predictions were performed on the training set (data set 1). Fig. 4 contains the results from the predictions of the true test set where the transfer model was created with data set 1 and then applied to data set 2. The same instrument A calibration was used. According to the figures, the performance of the transfer methods can be divided into 3 groups.

The first group contains a calibration developed with uncorrected spectra (UC 1) and another similar calibration but with certain wavelengths removed (WLS). Predictions with these two models resulted in large RMSEP and bias values.

The next group contains models resulting from MSC, SNV, 2nd derivative and PDS corrected spectra. Calibrations in this group have smaller RMSEP values then the previous group. The bias is quite large for the MSC, SNV and 2nd derivative corrections, while PDS seems to give a smaller bias then the other methods in these two first groups.

The third group contains models resulting from locally centered and uncorrected spectra (UC 2), 2nd derivative followed by 1 OSC component (Der + OSC), SNV followed by PDS (SNV + PDS), globally and locally centered 2 component OSC corrected (OSC 1, OSC 2) spectra. The RMSEP values are small for calibrations in this group. The UC 2 and Der + OSC models resulted in a bias close to zero while SNV + PDS gave a slightly higher value. The OSC 1 and OSC 2 models show a bias that is approximately twice as large as the bias for the SNV + PDS model. The OSC corrected models seems to be more biased than the other correction methods in group 3. This is probably due to the multiplicative bias [14], which is related to the 'regression towards the mean'.

The OSC bias could be reduced by fewer PLS-components in the calculation of the w^*. If only four PLS-components were used, the bias decreased to 0.004 while the RMSEP remained on the same level.

The locally centered model with no further treatment was performing well in group 3. There are,

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Fig. 7. Loadings. (a) The first three components for the MSC treated model, (b) first two components for the OSC treated model. Component numbers: 1, solid line; 2, interrupted line; 3, dotted line.

(a)

(b)
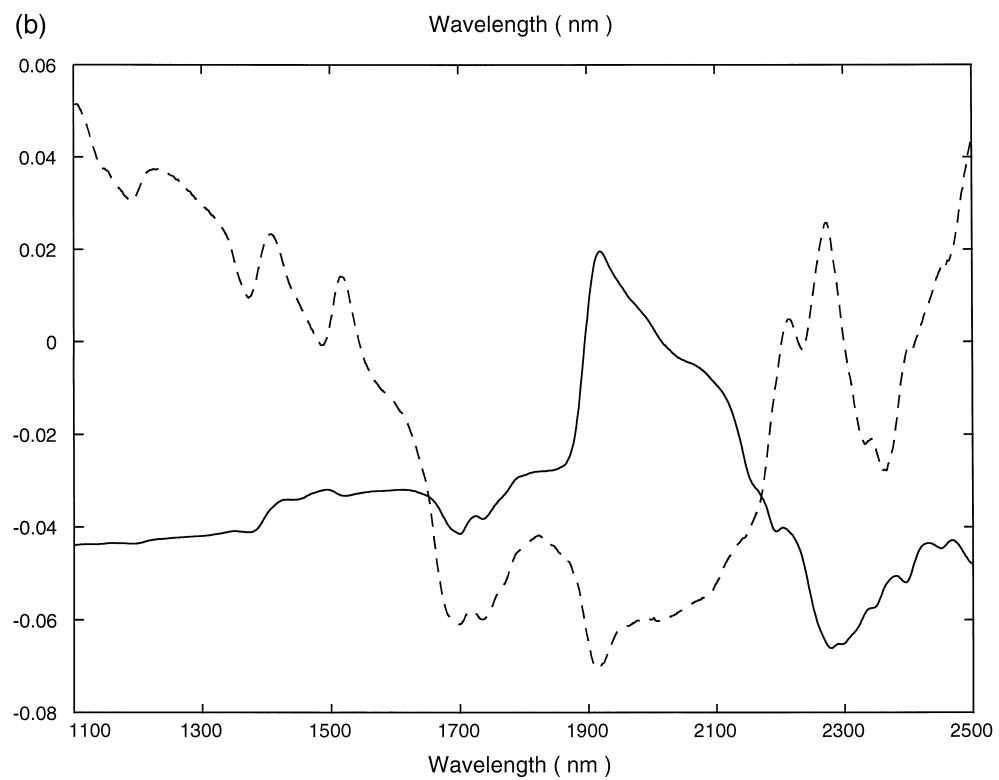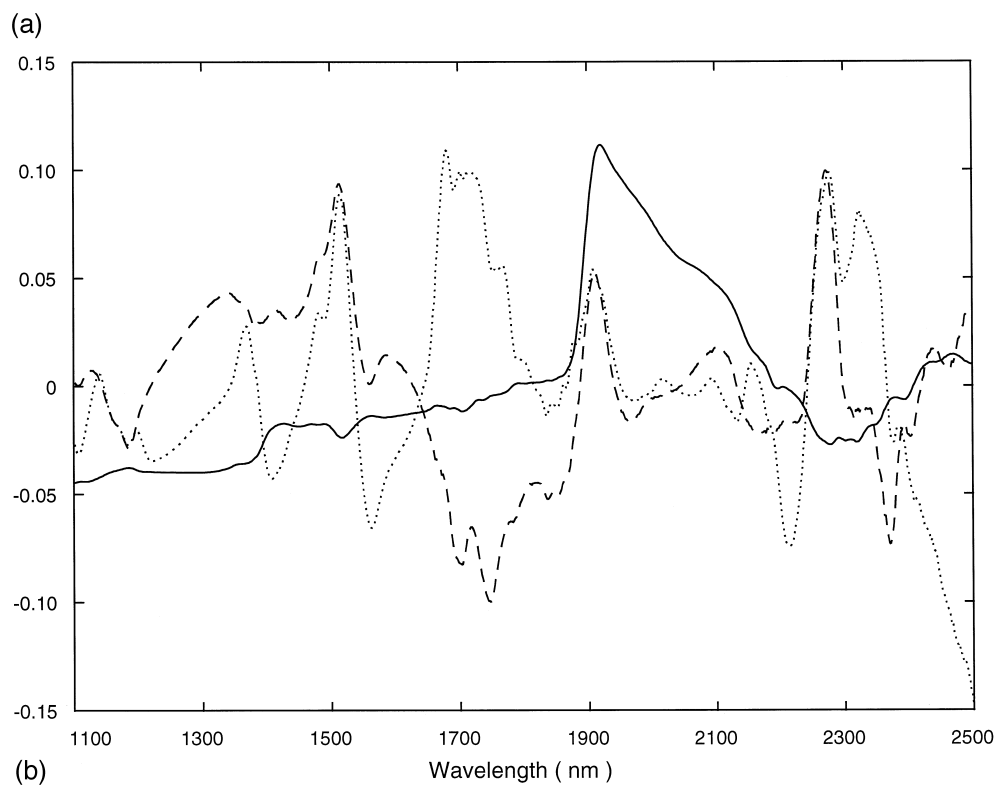
however, some problems with local centering only, since a representative average spectrum is needed. This average spectrum has to exist before the calibration can be used on a new target instrument. This means that more than a few spectra has to be run on the target before a UC 2 type transfer can be made. This calls for an independent way to generate some kind of instrument average that would possibly be easier to generate with a set of standards than with the actual samples.

For the calibration transfer test 3 the results are shown in Fig. 5. All spectra in data set 1 were used to define the transfer of spectra, and now both instruments A and B were included in the model. In this case the RMSEP and bias values were small for all the correction methods used in this paper. The results from this test show that, if we include samples from both instruments, the PLS-model in itself can compensate for the instrument variations. In some cases this may be the only solution available when the properties of the samples are changing rapidly and the samples become difficult to transport between labs. This is the case for the water content of samples if the vials are non-tight or opened often, since water is an abundant 'contaminant'. However, it would be easier to handle if a calibration could be made once and then used for other instruments with corrections involving as few extra measurements as possible.

The original calibration with NIR spectra versus Karl Fischer water content had an RMSEP of ≈ 0.1 wt./wt.%. All transfer methods in group three above and all calibrations including both instruments had a lower RMSEP between the instruments. This means that for this type of water content measurements it would not be difficult to find a transfer method that holds. One of these methods was the OSC, but the OSC correction was not the best in this case.

4.2. Features of orthogonal signal correction

Indications about the function of OSC for removal of instrument specific features, were obtained by comparing scores, loadings, and *y*-residuals from uncorrected calibrations and calibrations after MSC or OSC. These results are based on the calibration transfer test 3 with the two instrument calibration.

In Fig. 6(a) the score plot for the first two PLS-components of a 4-component model based on MSC corrected spectra shows two groups containing spectra from the two instruments. This indicates that the MSC was not able to remove the instrument difference. In contrast to this, the 2-component PLS-model after a 2-component OSC, does not show the instrumental variation in the score plot (Fig. 6(b)). This means that OSC could remove instrumental variation in this data set with more success than MSC.

When studying the loading plots in Fig. 7, we observe that in the first component the loadings is very similar for both the MSC and the OSC treated models. In the MSC treated model, 3 additional components were required to model the remaining **Y** and the instrumental variation. In the OSC model treated with two OSC-components, only one weak additional component was required. Wood's anomaly at 1500 nm was less modelled in the OSC model than in the MSC model. This means that the OSC was able to remove the structure from the anomaly better than the MSC.

Since an OSC component loading vector (w^* in Eq. (10)) is combined from several PLS-loading vectors to produce a set of regression coefficients towards the MLR type, it is relatively difficult to interpret [16]. A full interpretation involves the expansion of all the 15 PLS-components generated between the Eqs. (9) and (10) above.

Fig. 8 shows the *Y*-residuals versus *Y*-predicted for a MSC treated model and a OSC treated model. With the MSC, the residuals have a structure with positive residuals at low and high predicted water contents and negative residuals for values between 2 and 3 wt./wt.% water. After OSC, the model does not show this pattern, and the residuals are more randomly distributed. This indicates that OSC can correct mild non-linearities in spectra. Thus it is possible to work with full spectra in the calibration, avoiding to use e.g., variable selection as a first step.

To show the spectral changes during OSC, spectra from two batches measured in duplicate on both instruments are shown in Fig. 9 after (a) no correction, (b) 1 OSC component removed and (c) 2 OSC components removed. The spectra were locally centered before correction. The four spectra with a large positive peak at ≈ 1900 nm originate from the same vial and the other four spectra from another vial. For each removed OSC component the spectra become more similar to each other. This is caused by the removal
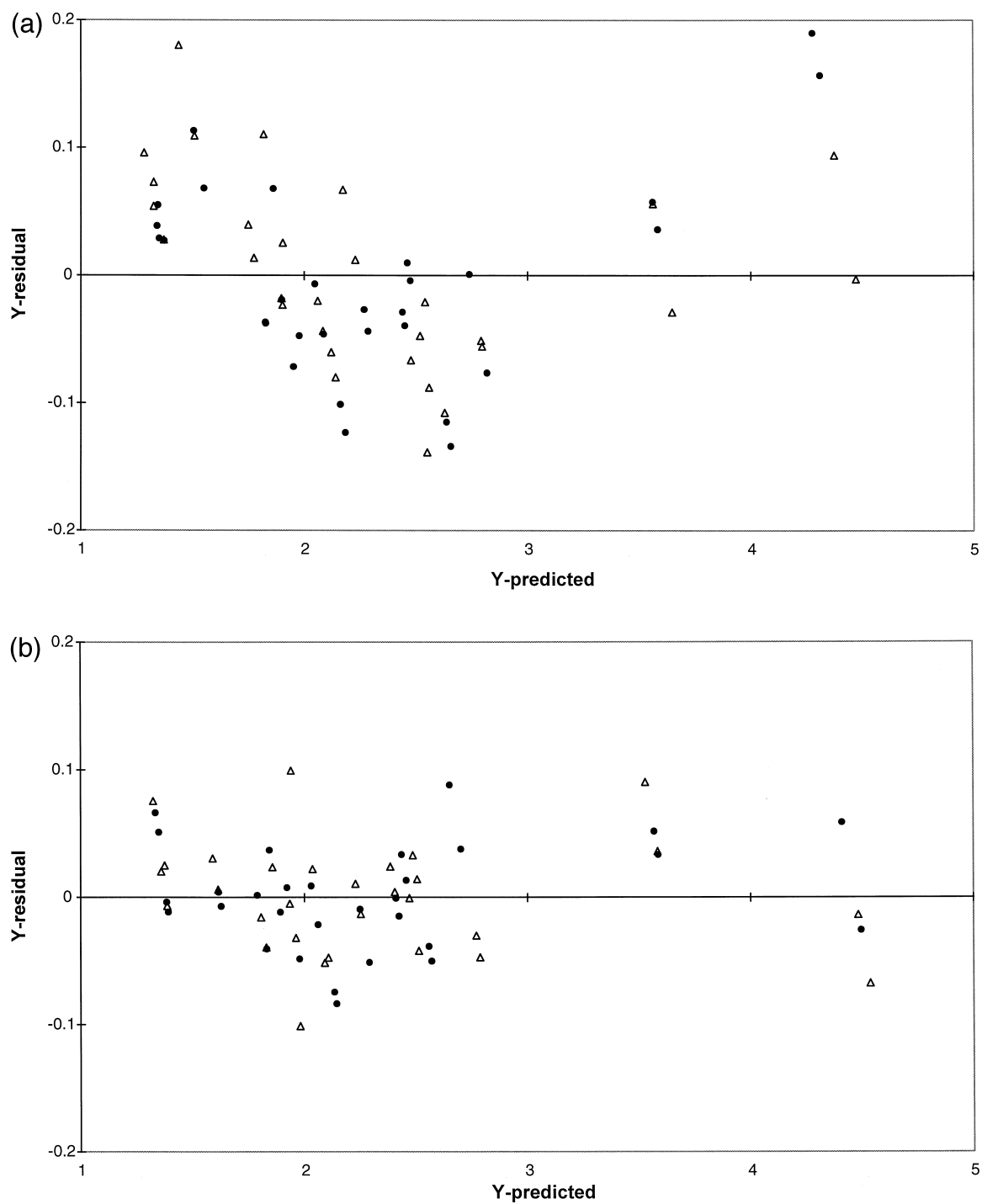
Fig. 8. *Y*-residuals versus *Y*-predicted for (a) MSC treated model and (b) OSC treated model. Triangles represent instrument A, filled circles represents instrument B.
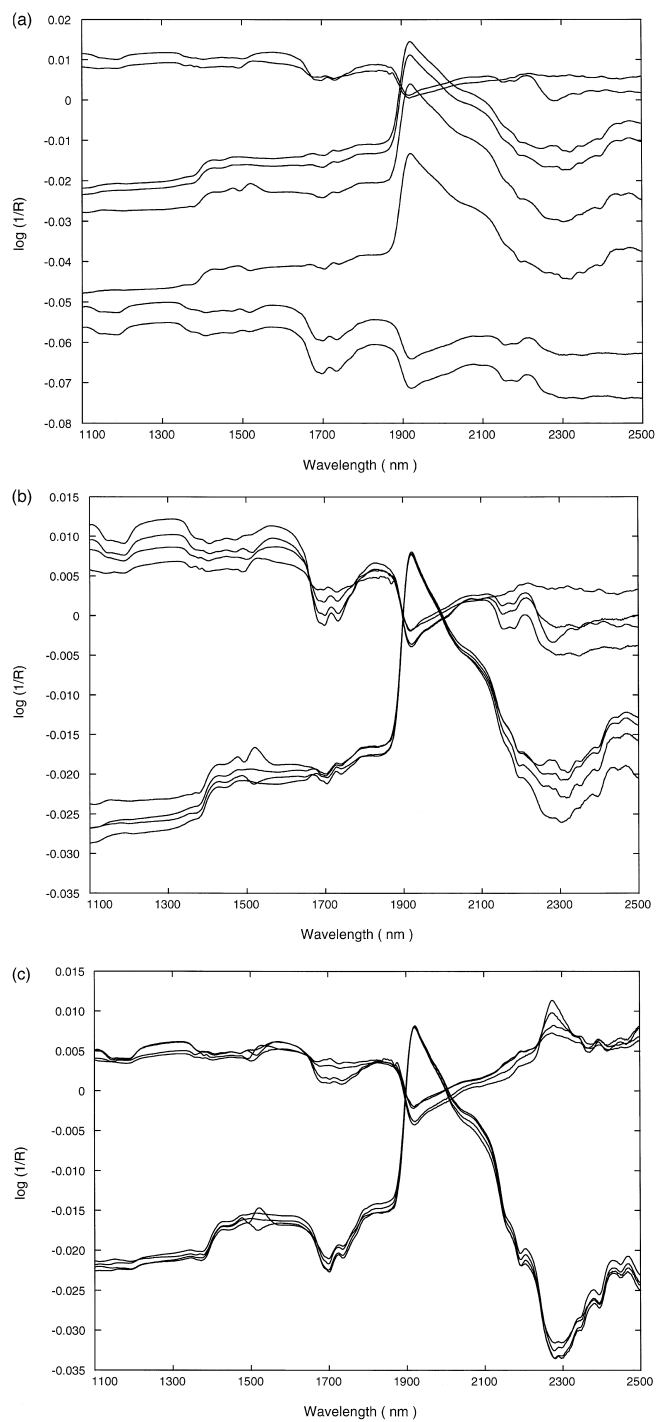
Fig. 9. Replicated spectra from two samples at both instruments (data set 1), (a) Locally centered spectra. (b) One OSC-component. (c) Two OSC-components.

of variations in the spectra that does not correlate with **Y**. After excessive use of the OSC by taking 20 OSC components, the spectra became almost identical. However, 20 OSC components should not be used because of problems due to overfit.

5. Conclusions

Local centering performs very well compared to the more sophisticated signal correction methods for these data sets. The reason for this is that the two instruments are quite similar and the difference in the resulting spectra is mainly a linear shift. In a situation like this, all methods with local centering performs well even without correction, because the local centering takes in account the linear shift of the spectra. The only methods performing correctly without local centering were OSC and SNV + PDS. In the OSC case both global and local centering gives the same results, indicating that OSC takes care of the linear shift. When using spectra from both instruments in the calibration set, all the signal correction methods perform equally well and no signal correction seems necessary. This is because PLS models the instrumental differences.

The OSC could remove parts of the instrumental variation, and the **Y**-residuals were more randomly distributed than for the other methods. When corrected with other methods they showed a slight curvature. These properties are promising and should be investigated further with other data sets. As this study was performed on similar instruments, we should continue to compare these methods with more different instruments.

6. Future work

This work only concerns data sets with the same samples for both instruments. Data sets spanning a wider range of samples and instruments need to be analysed. Additional preliminary tests of calibration transfer with no correction, local centering, PDS and OSC between an FT-NIR and a dispersive instrument were made as a response to one of the review-

ers. In this case the samples were a calibration set and a test set for the concentration of an active substance. This involved the conversion from reciprocal cm and a re-interpolation to even wavelength intervals of the FT-NIR spectra. In this case the uncorrected spectra gave an RMSEP that was 10–15 times larger than for the corrected spectra. Surprisingly, the same relative pattern as for the transfer test 2 emerged, where the local centering performed well together with the PDS and the OSC corrections.

During this work the modelled variation in **X** has been used together with a verification of the *y*-orthogonal properties of the subtracted OSC components. Since good balance between the number of OSC-components and the number of components in the final calibration model has to be maintained, there is a further need for the investigation and development of diagnostic tools for the determination of the optimal number of OSC components.

Another topic that would be interesting to investigate is other orthogonalisation algorithms that also take into account the explicit knowledge about on which instrument the spectrum was measured in combination with other known chemical differences. This might be done by combining the present OSC algorithm with discriminant PLS.

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