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Forage Calibration transfer from laboratory to portable instruments: challenges and applications

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Outline

- There is a problem (Lab bench → Handhelds)
- I’m not satisfy of results
- Any Idea?

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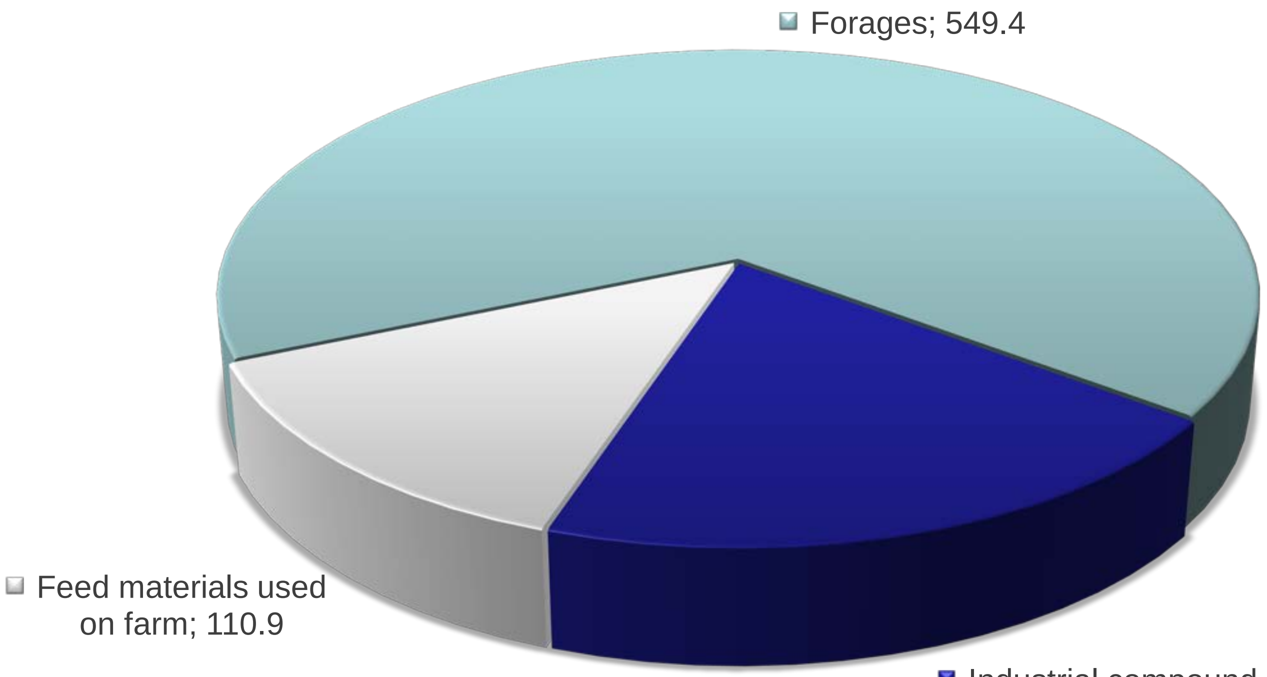
Europe Feed and Forage market

Livestock sourcing in feed in the EU+UK (825 mt. in 2020)



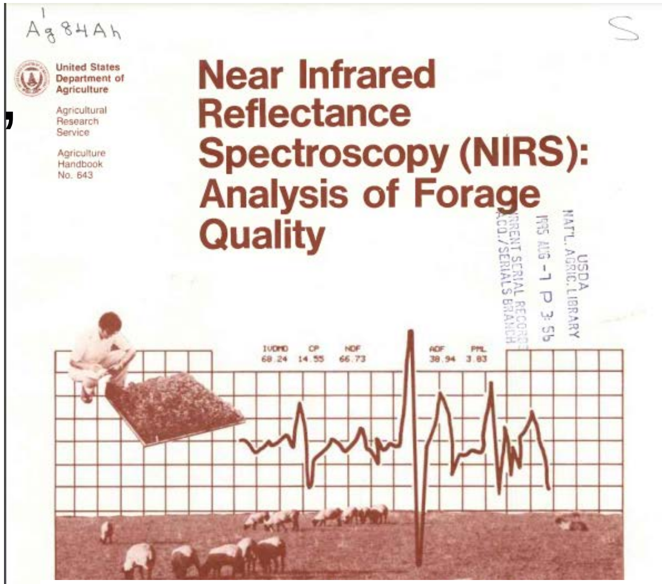
Source: FEFAC, DG AGRI

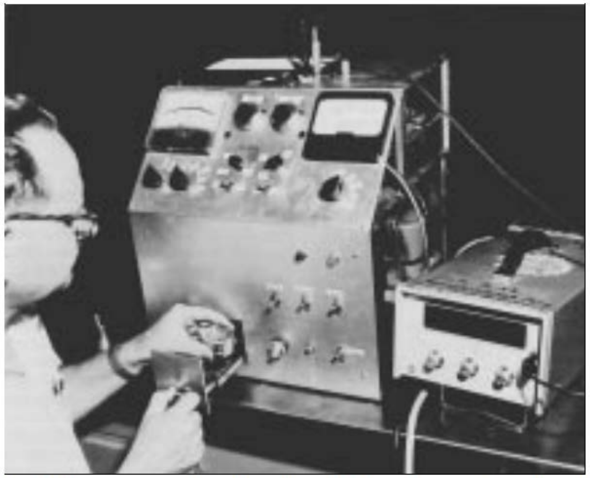
mt = million tonnes

When it all (NIR speaking) started

- Composition (protein, fat, moisture, starch, Energy, …..)
- Biological properties (Digestibility, palatability)

- Since the early time, NIR has established itself as the analytical method of choice for farms, feed company, feed and forage trading





Karl Norris operating the first NIR analyser for oil and soya beans (1968).

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Laboratory NIR instruments

€€€€€€€€$$$$$$$$$$

Traditional Lab Challenges

- Too slow!!
  - Sampling
    - Taking the sample to a lab
      - Preparing the sample (drying & grounding)
        - Preparing the sample in a scanning cup
          - Selecting the appropriate calibration
            - NIR Scanning and predicting
              - Getting results back to the user

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At farm applications

- Need to take the NIR to the samples
  - To have rapid answers
  - Implement immediate corrections when needed

- Need to have the technology more accessible
  - Lower cost

Portables/handhelds

Take the instrument to the product to analyze

- **Sampling**
  - ~~**Taking the sample to a lab**~~
    - ~~**Preparing the sample (drying grounding)**~~
      - ~~***Preparing the sample in a scanning cup***~~
        - **Selecting the appropriate calibration**
          - **NIR Scanning and predicting**
            - **Getting results back to the user**

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Portable instruments

Fairy tales….??

Calibration transfer - Standardization

- There are different ways to transfer calibration (Fearn 2001):

1. Creating a robust calibration 'insensitive' of the differences between instruments
2. Adjust the results (Slope and Bias) using the same prediction model
3. Adjust the spectra (standardization)

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1 Laboratory vs 3 Handhelds

LAB = Foss6500 ~50000€

DA = Diode Array ~ 15000€

DLP = Dig. Light Processing ~ 3000€

SW = Short Wave ~ 300€

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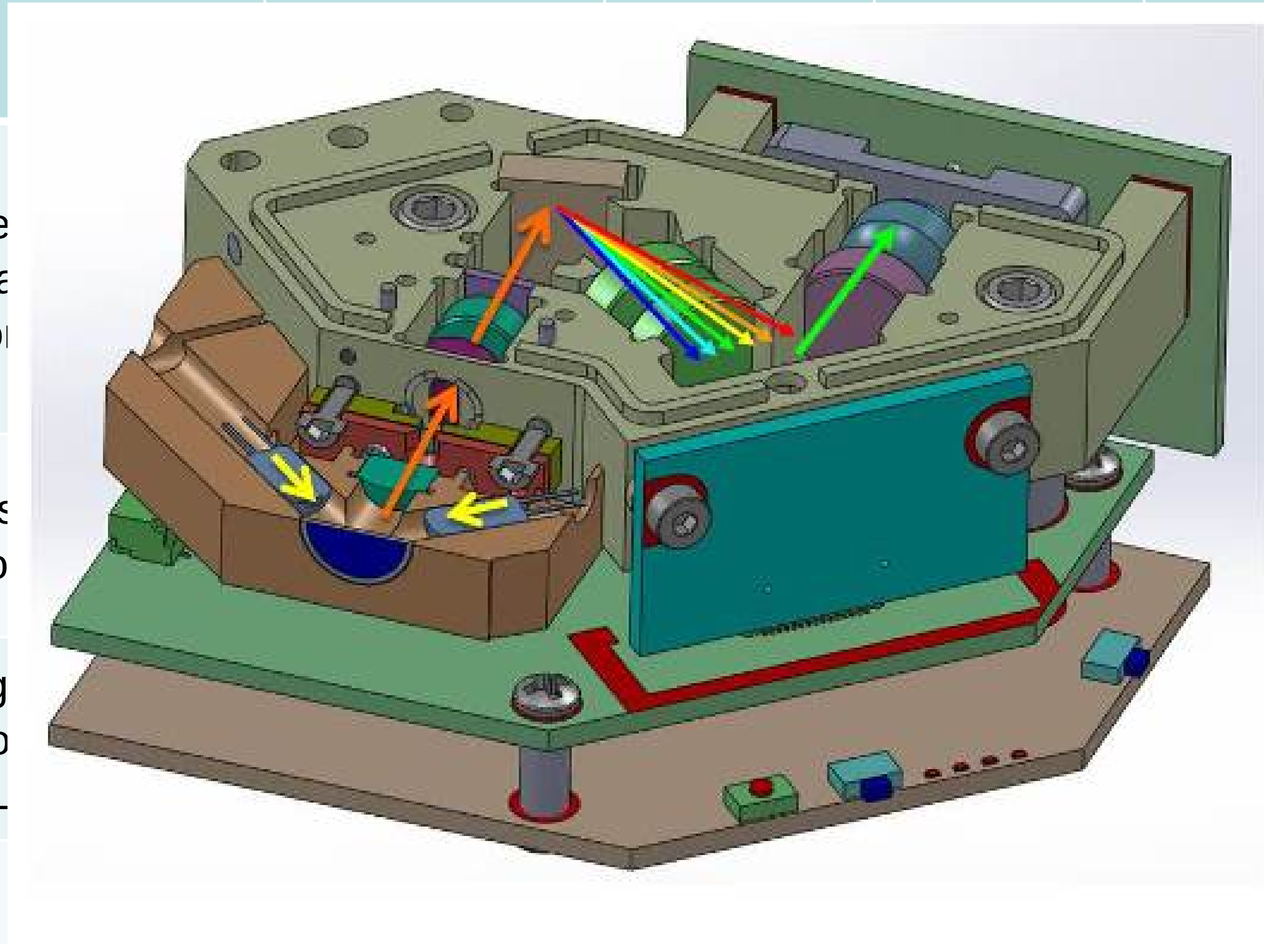
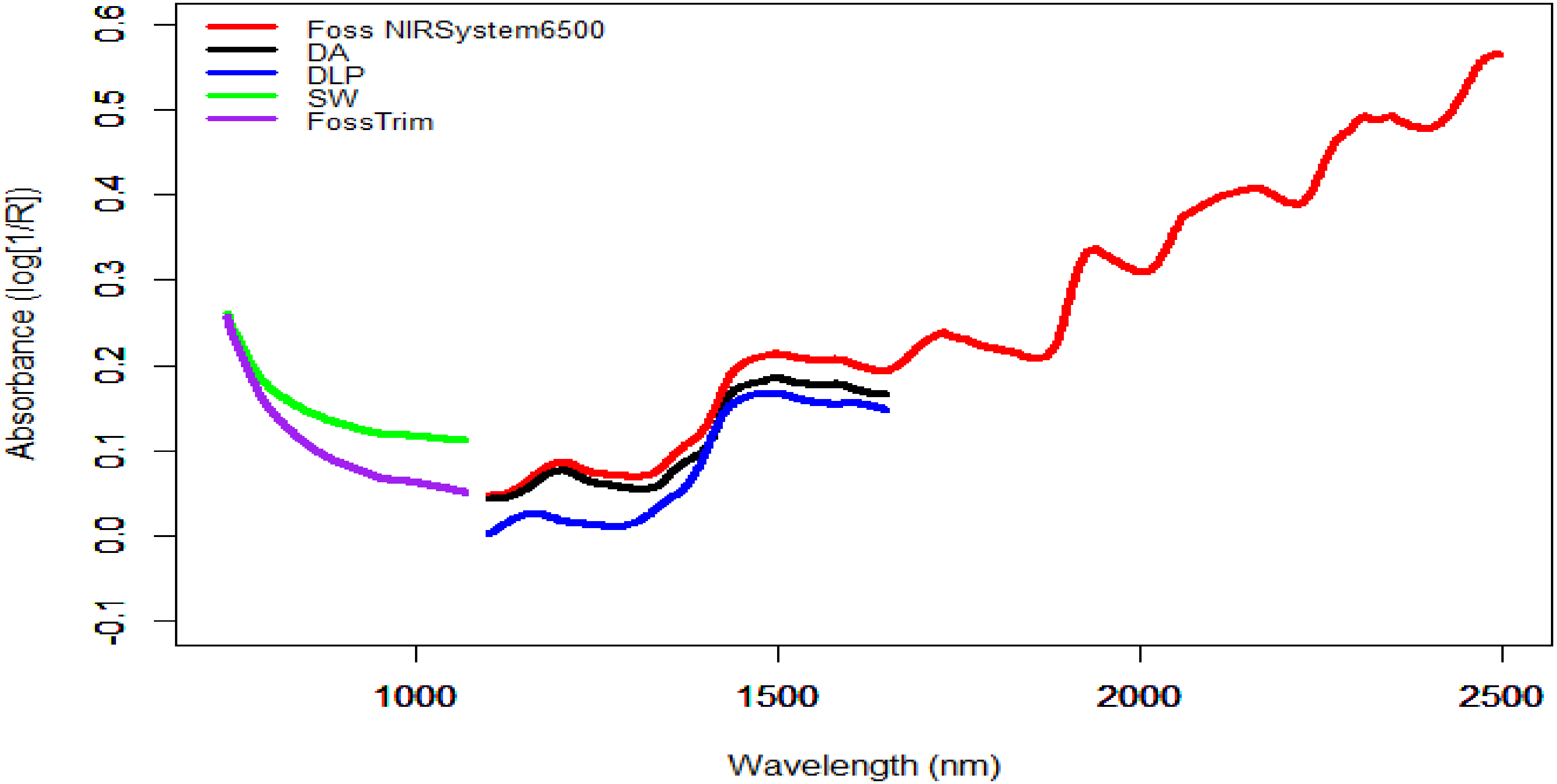
Features of the instruments

Instrument	Technology	Spectral range,	Sample	Scan Area	Number of	
LAB FOSS NIRSystem 6500	Pre Sca mo				ns	
DA AuroraNir	Pos Dio				s of 2s ximately ectra)	
DLP NIR-S-G1	Dig Pro (DL				ns of 3s ximately ctra)	
SW SCiO	unknown	740-1070, 12	Contact	(6x9mm)	3 scans	



Average Spectra



Forage samples

- Samples were from 8 agronomic trials at Cornell University (Dr. Jerry Cherney)
- Dried (60 °C) and ground (1mm, Wiley

Trial no.	Study	Year		Alfalfa, n.	Grasses, n.
15-45	1	2015	Calibration	100	94
15-85	2	2015	Calibration	40	33
16-67	3	2016	Test-set	88	54
16-69	4	2016	Test-set	63	63
16-91	5	2016	Calibration	83	83
16-92	6	2016	Calibration	52	60
17-68	7	2017	Calibration	60	48
17-93	8	2017	Calibration	126	81
Total				612	516

Berzaghi et al., 2021

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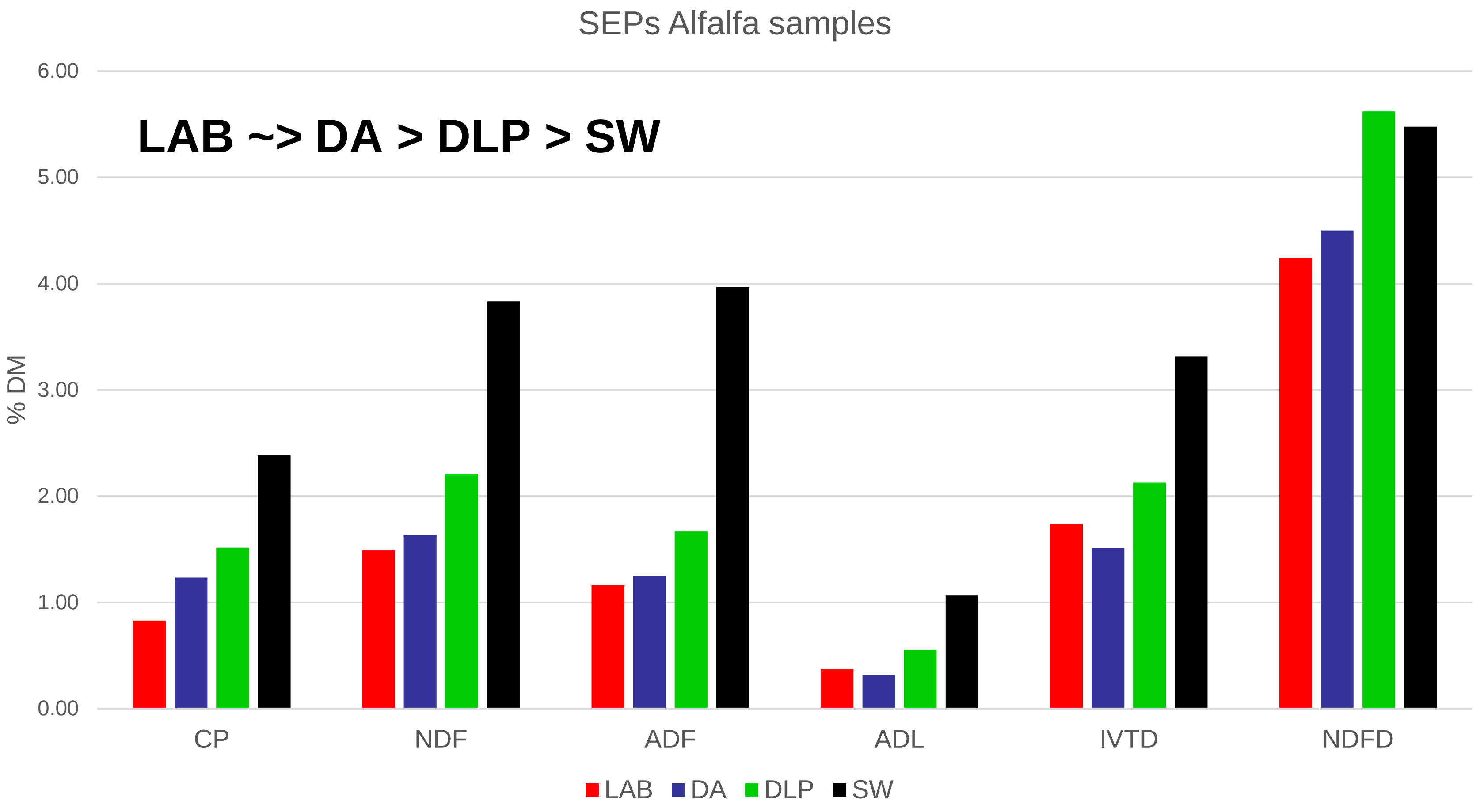
Comparing performances



Berzaghi et al., 2021

Goal

Slave **Transfer to handhelds** **Masters**

LAB calibration developed over the years

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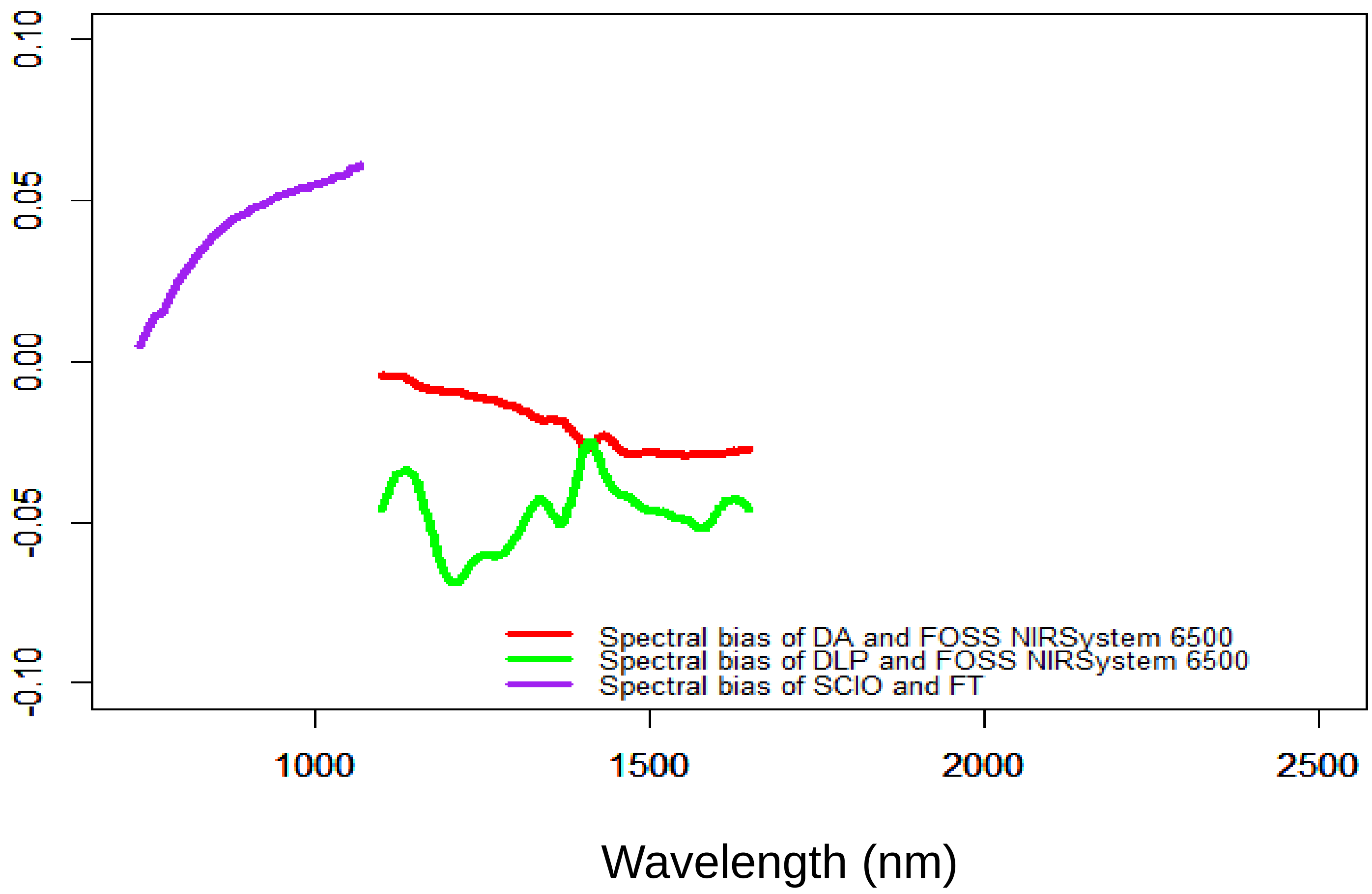
Average difference from LAB spectra



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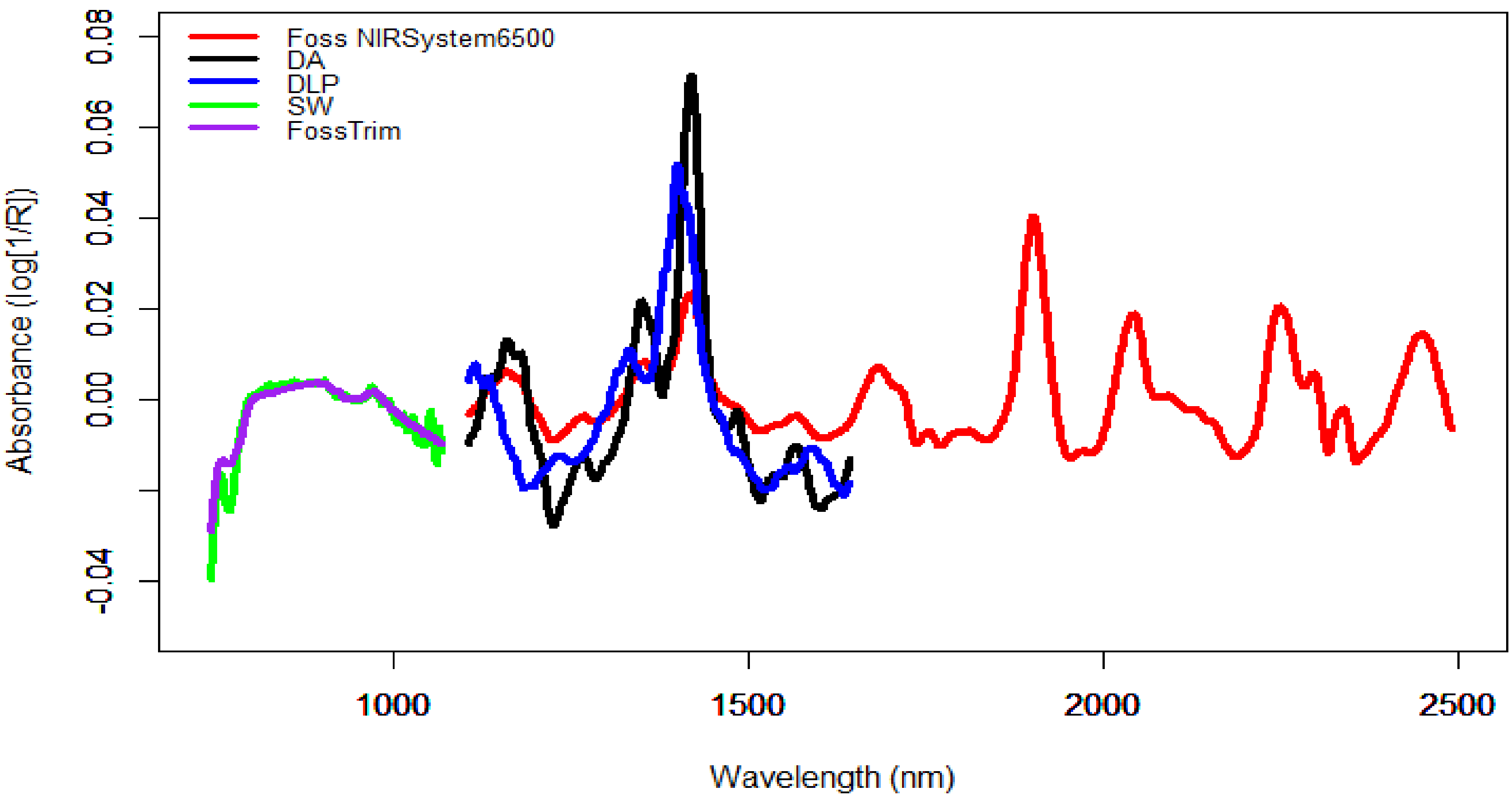
Spectra after math treatments

SNV, Detrend, SG 1d, 7gap



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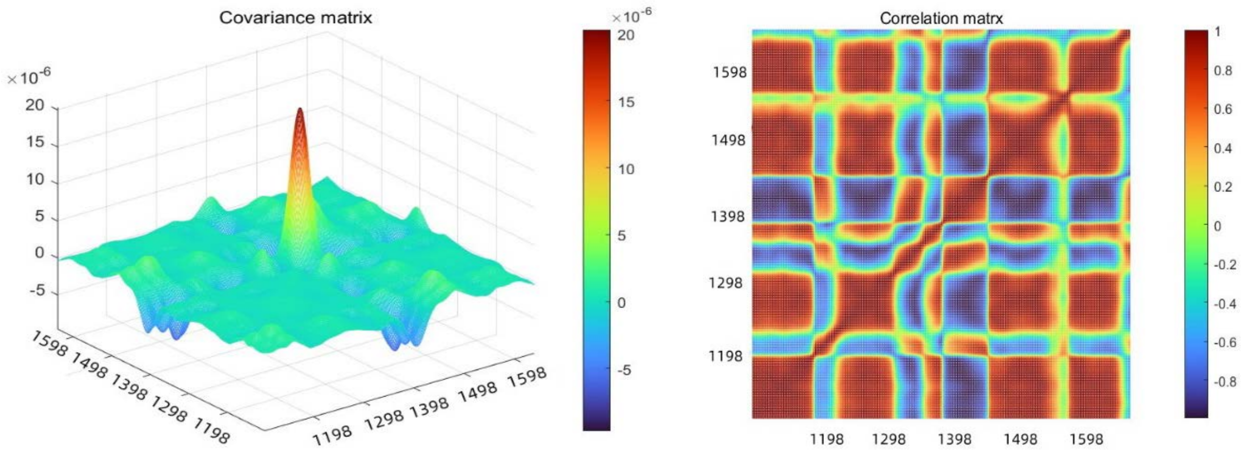
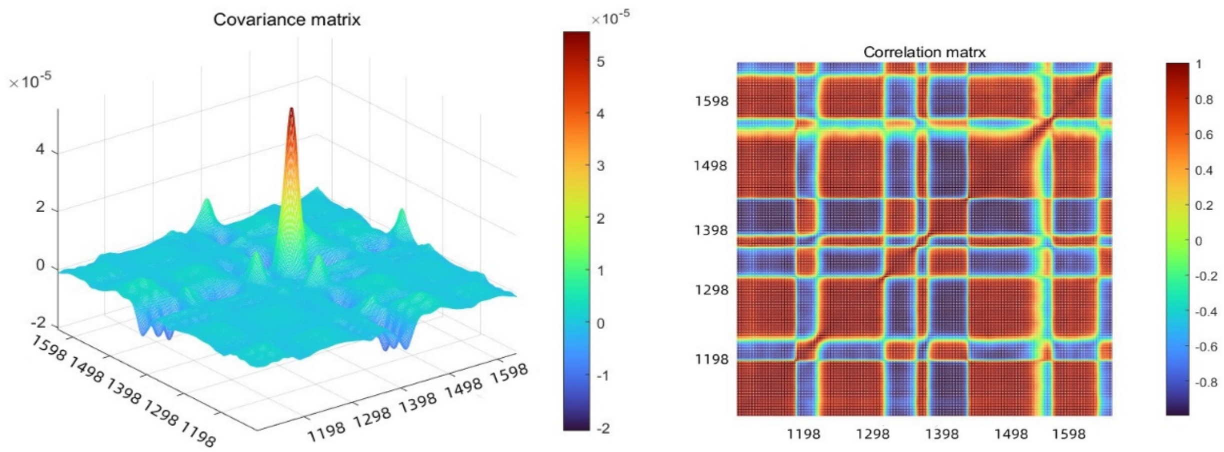
Hardware differences

SNV, Detrend, SG 1d, 7gap



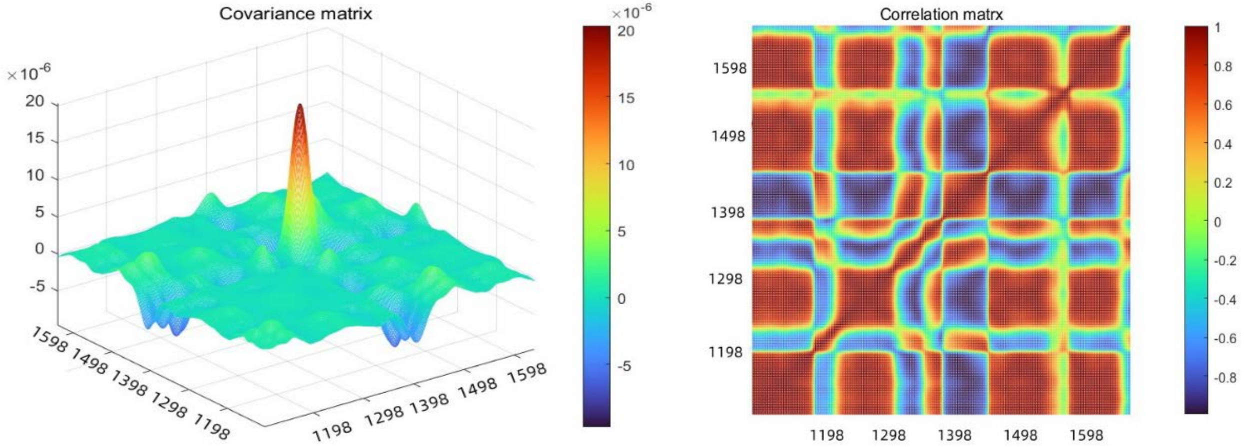
LAB (1100-1650 nm)



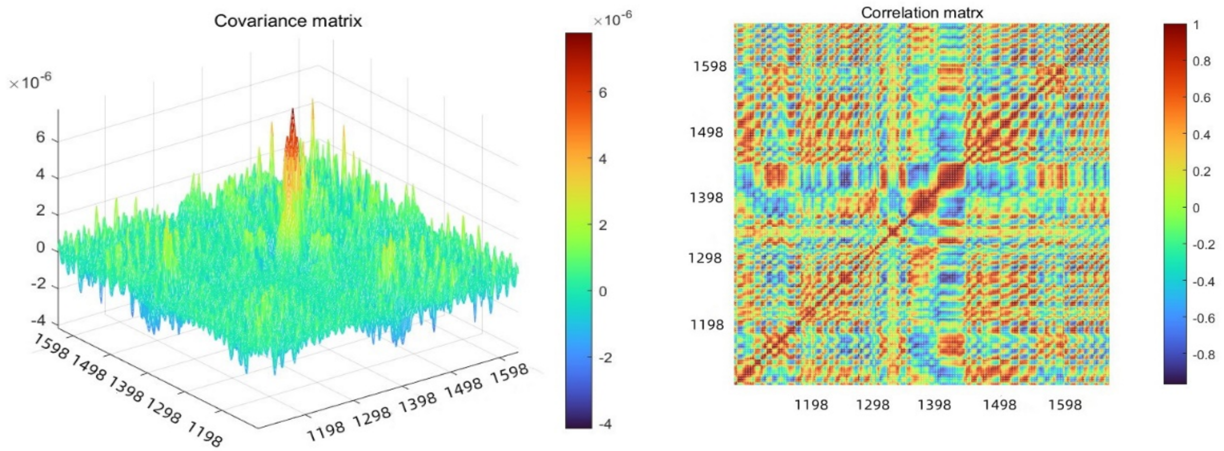
DA (1100-1650 nm)

Hardware differences

SNV, Detrend, SG 1d, 7gap



LAB (1100-1650 nm)



DLP (1100-1650 nm)

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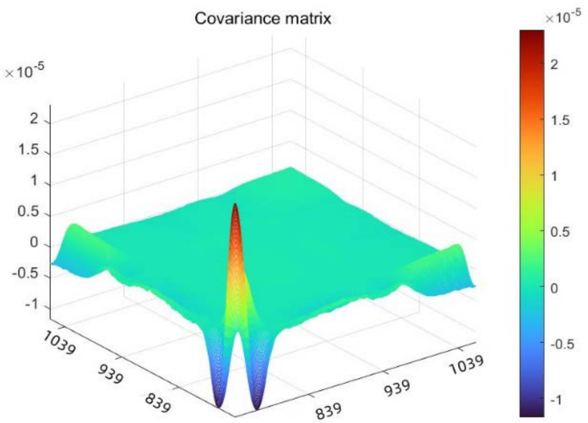
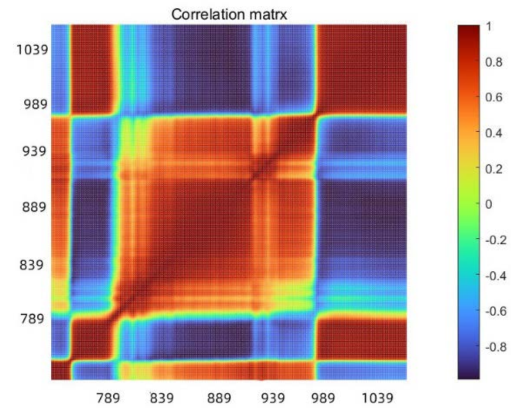
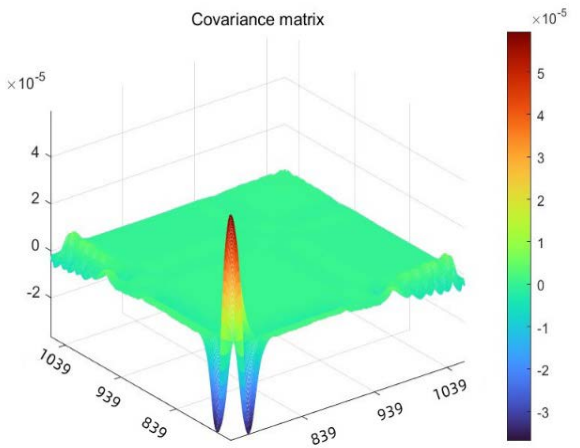
Hardware differences

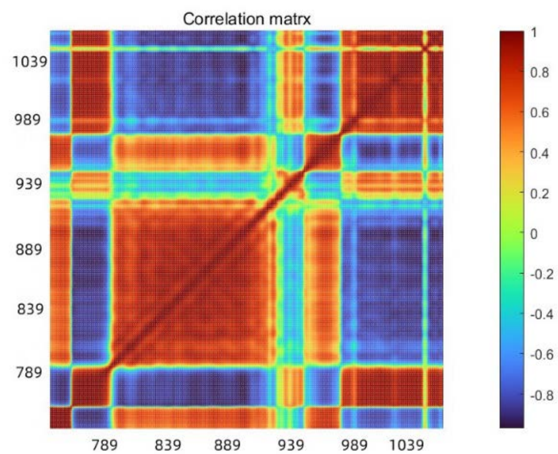
SNV, Detrend, SG 1d, 7gap





LAB (740-1070 nm)





SW (740-1070 nm)

Calibration transfer

Spectra correction:

- **Spectra Bias Correction**: simply apply the average spectral difference to the Master instrument
- **Piecewise Direct Standardization**: 1 Comp, Windows 3 datapoints (RNIR)
- **Shenk & Westerhaus**: WinISI

Inoculation

- Adding “real spectra and chemistry of Master instrument AFTER Spectra correction

Spectra correction challenges

- All instruments must scan the same samples, possibly untouched
- Sample presentation may affect spectra
  - Foss samples are placed in ring cup cuvette
  - The same cuvette could not be scanned on the DLP
  - Instruments were at different locations and spectra were collected at different times with possible changes of samples

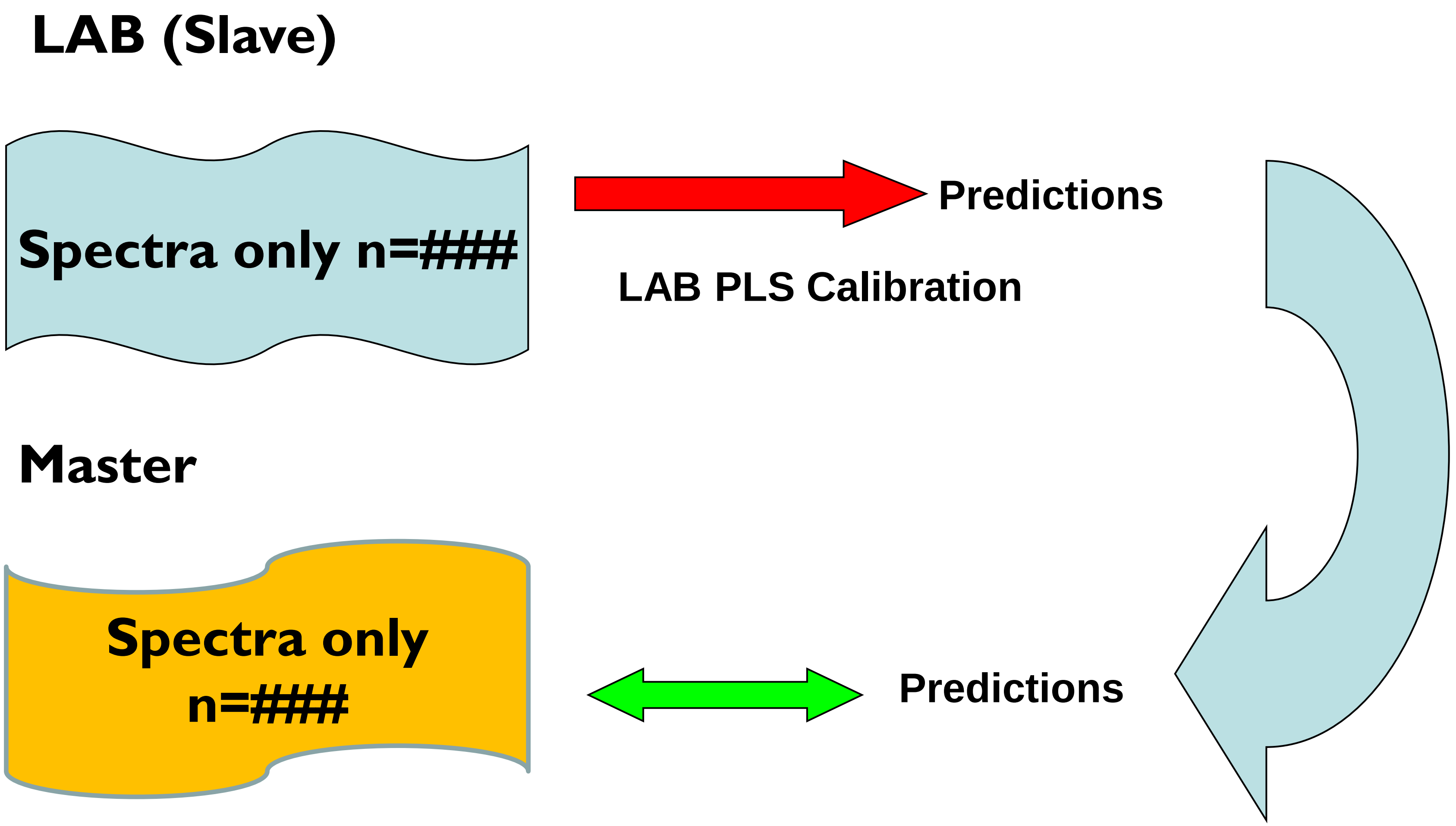
Using prediction as reference values

- What about using NIR prediction to develop a calibration for a new instrument? ☺

- Isn't it cheating? ☹

- Or is it a legitimate use of prediction data?

Using prediction as reference values



Using prediction as reference values

Master

Spectra and ‘chemistry’ n=###

PLS1

$$\text{Constituent}=\beta_0+\beta_1+\beta_2 \ldots\ldots+\beta_n$$

Using prediction as reference values

- Advantages
  - Cheap and quick
  - Doesn't involve complicated chemometric
  - Can be used for instrument with different wavelength
- Disadvantages
  - Still need to scan the same samples on both Master and Slave
  - It will be easier to overfit new Master PLS models

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Forage samples

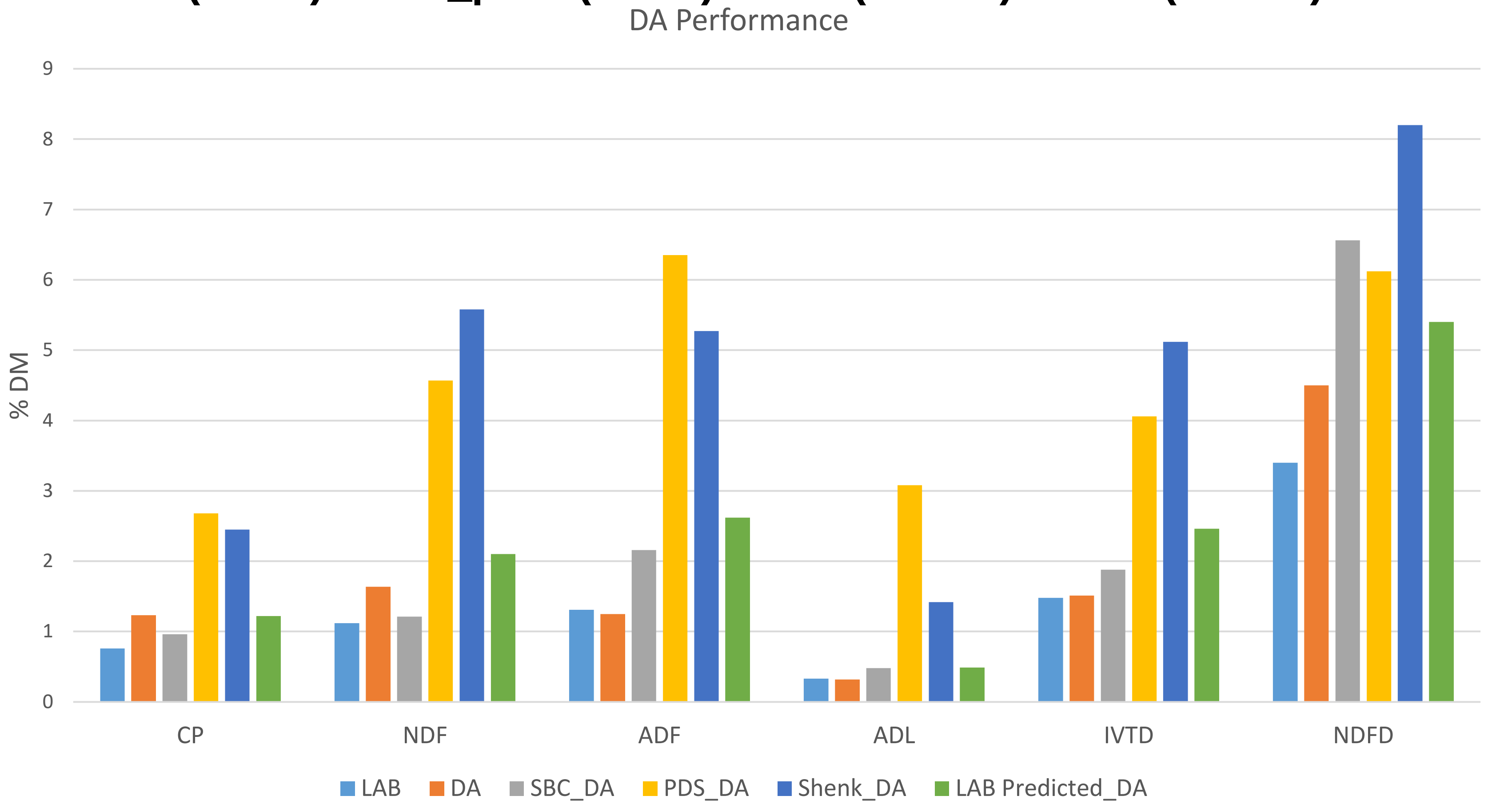
Samples were from 8 agronomic trials at Cornell University (Dr. Jerry Cherney)

Trial no.	**Alfalfa, n.**	**Grasses, n.**
Total	612	516
LAB Calibration	295	285
Standardization	40	33
Test-set	151	117
Inoculation	42	42
LAB NIR predictions	124	114

CP = Crude Protein; ADF = Acid Detergent Fiber; NDF = Neutral Detergent Fiber; IVD = In-Vitro True Dry matter Digestibility; NDFD = NDF digestibility

DA SEPs Alfalfa

SBC (+26%) <LAB_pred (+36%) <PDS (+157%) <S&W (+168%)



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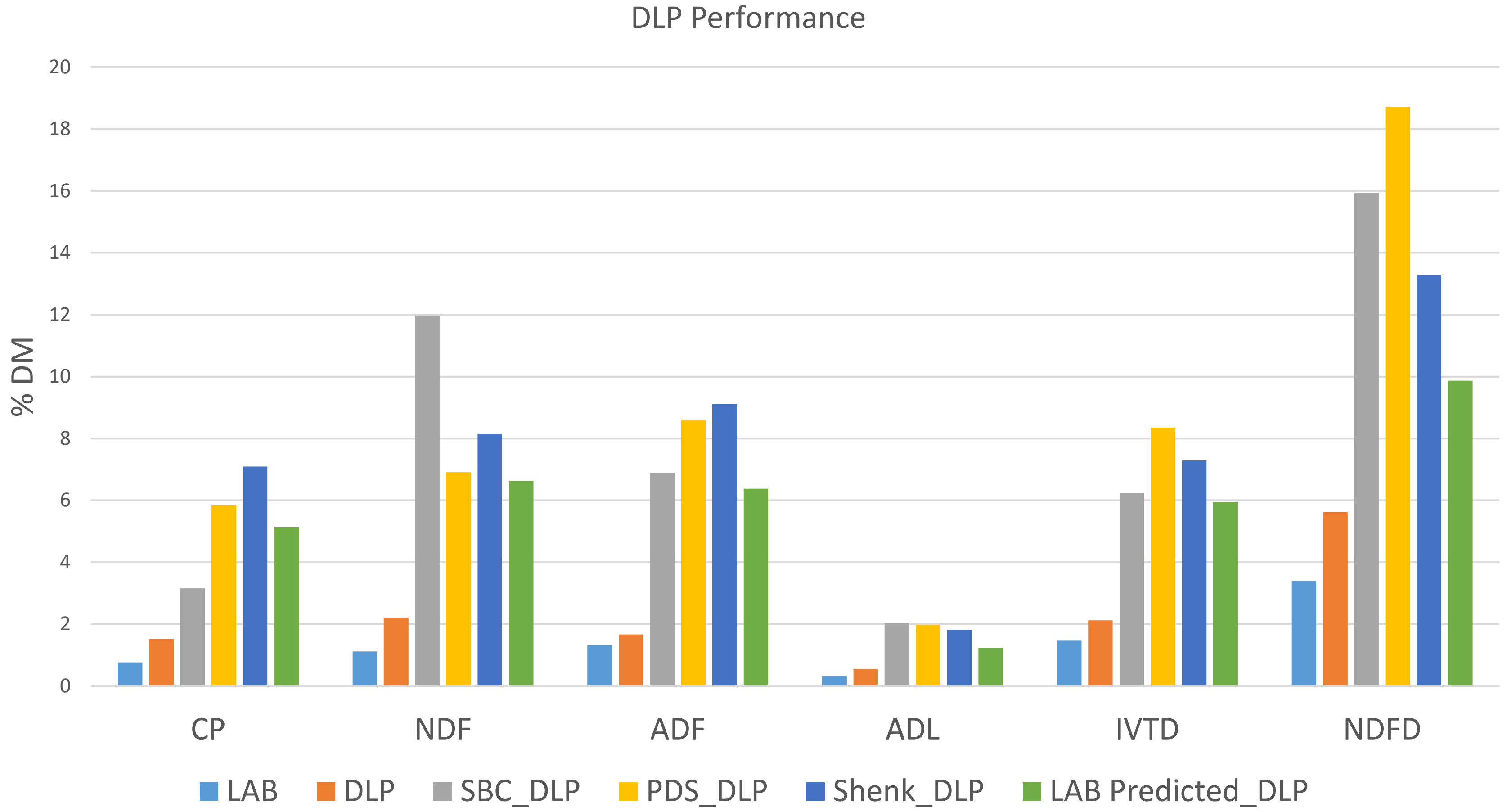
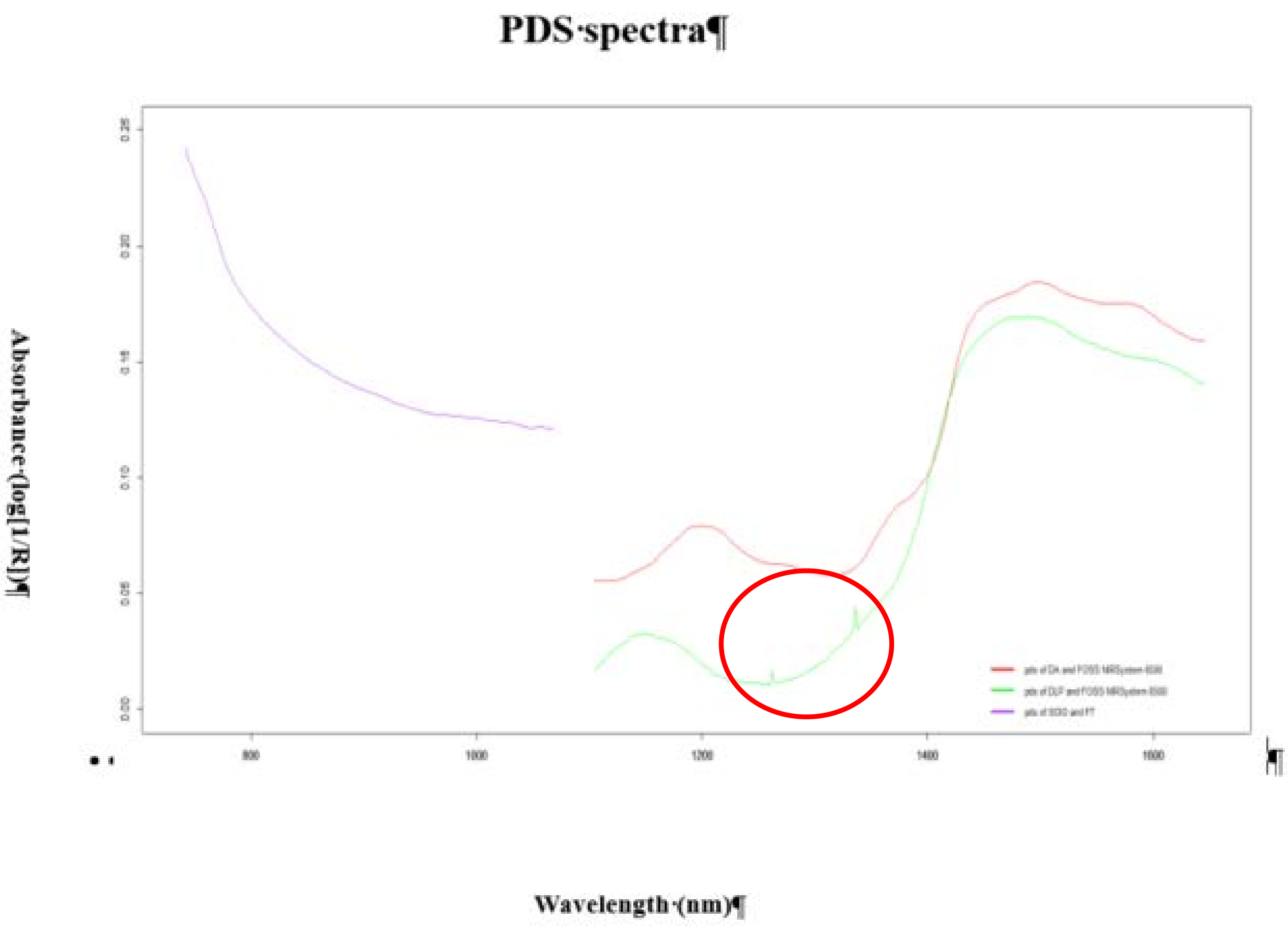
DLP SEPs Alfalfa

LAB_pred (+157%) <SBC (+237%) <S&W (+241%) <PDS (+268%)



PDS spectral artifact



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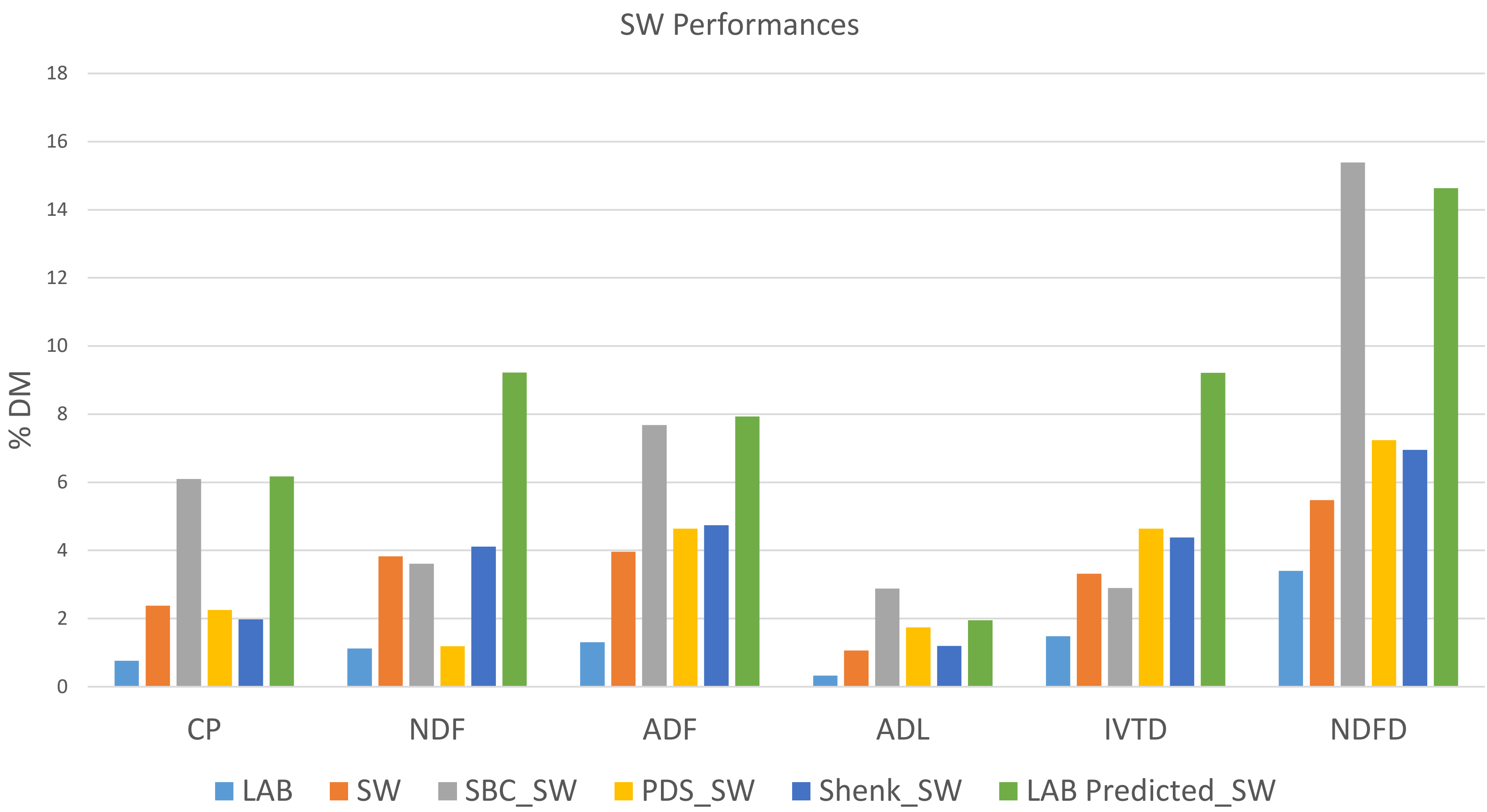
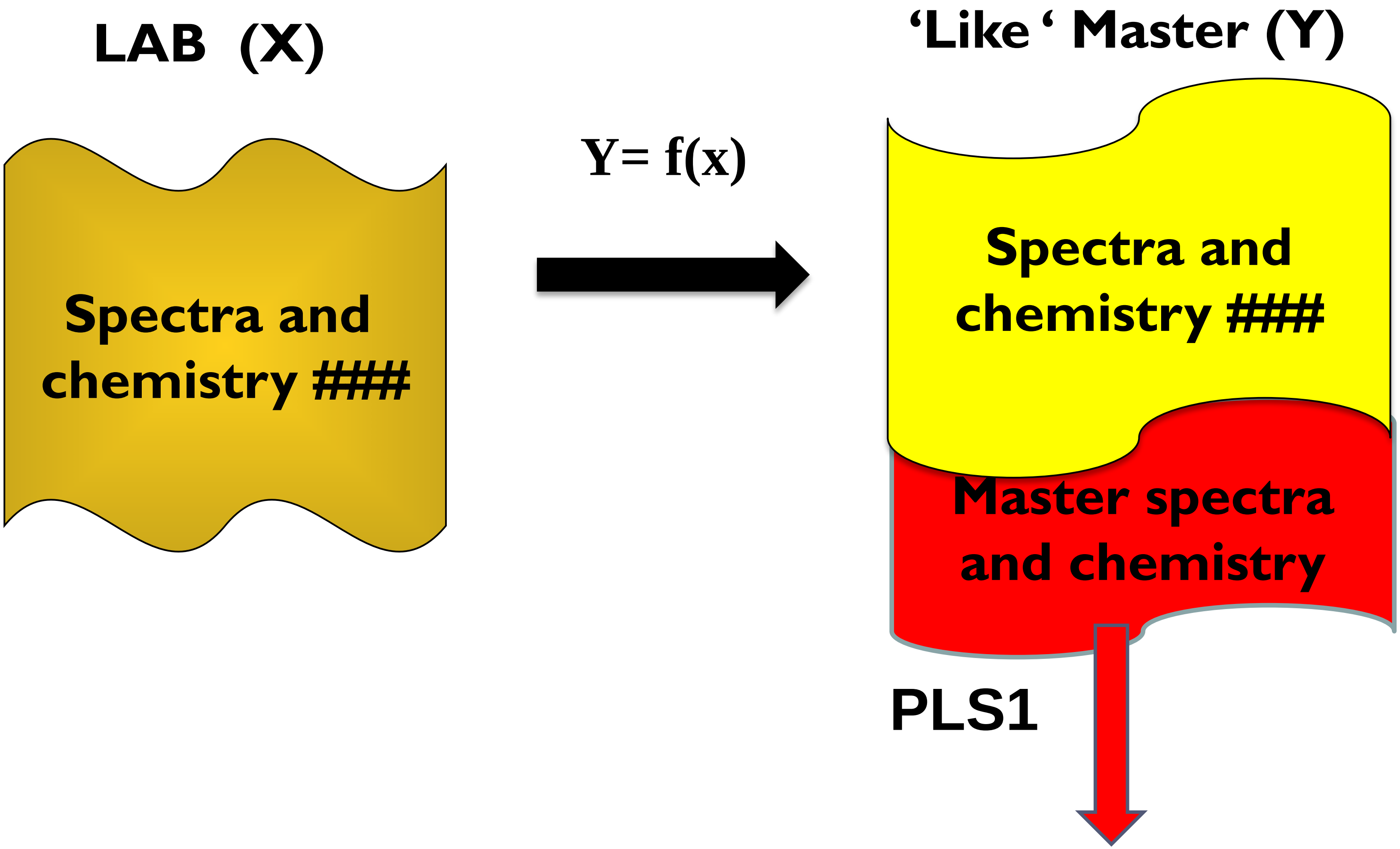
SW SEPs Alfalfa

PDS (+8%) < S&W (+16%) <SBC (+92%) < LAB_pred (+145%)



Calibration transfer - Standardization + updates



$$\text{Constituent} = \beta_0 + \beta_1 + \beta_2 \ldots\ldots + \beta_n$$

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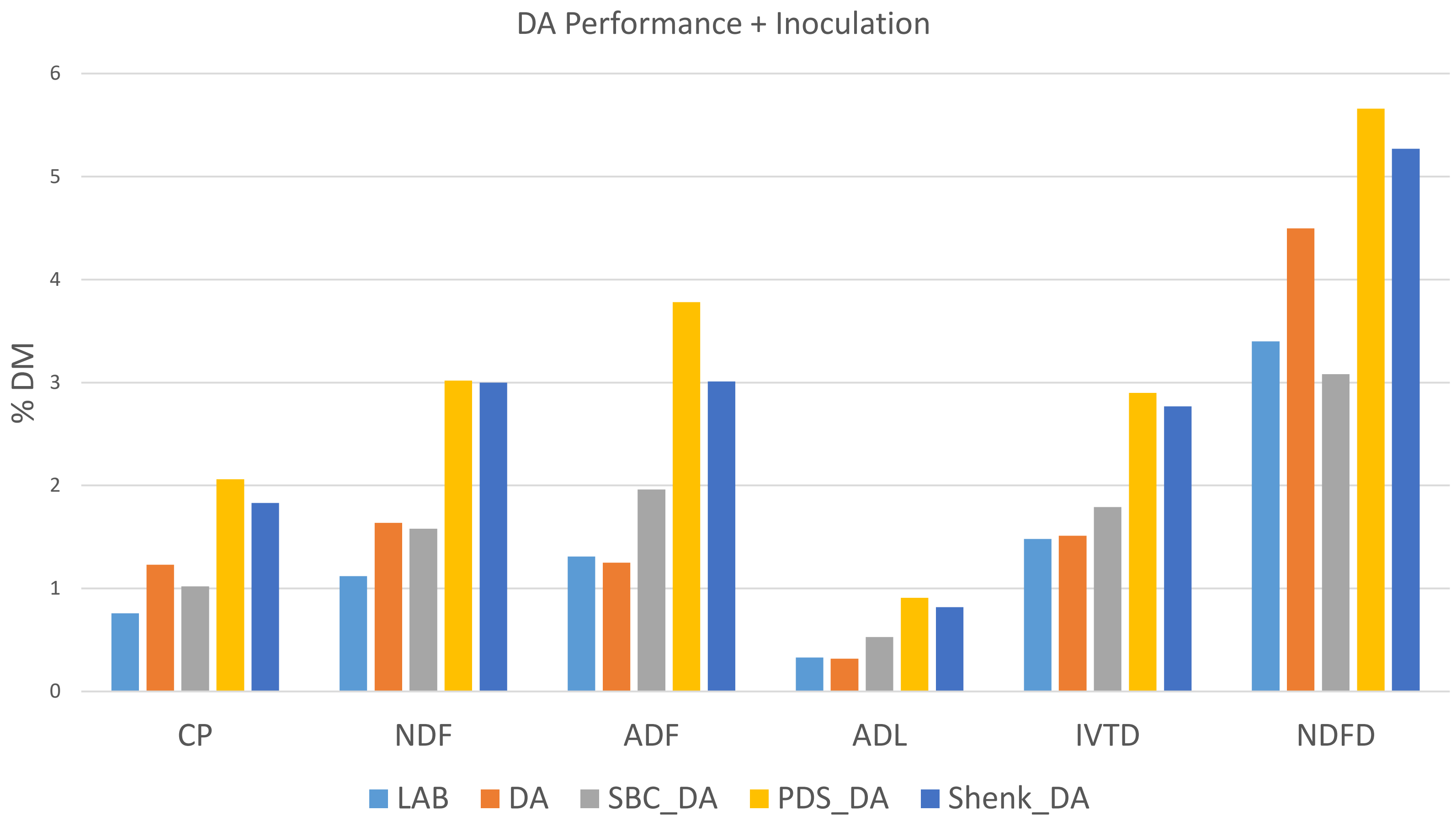
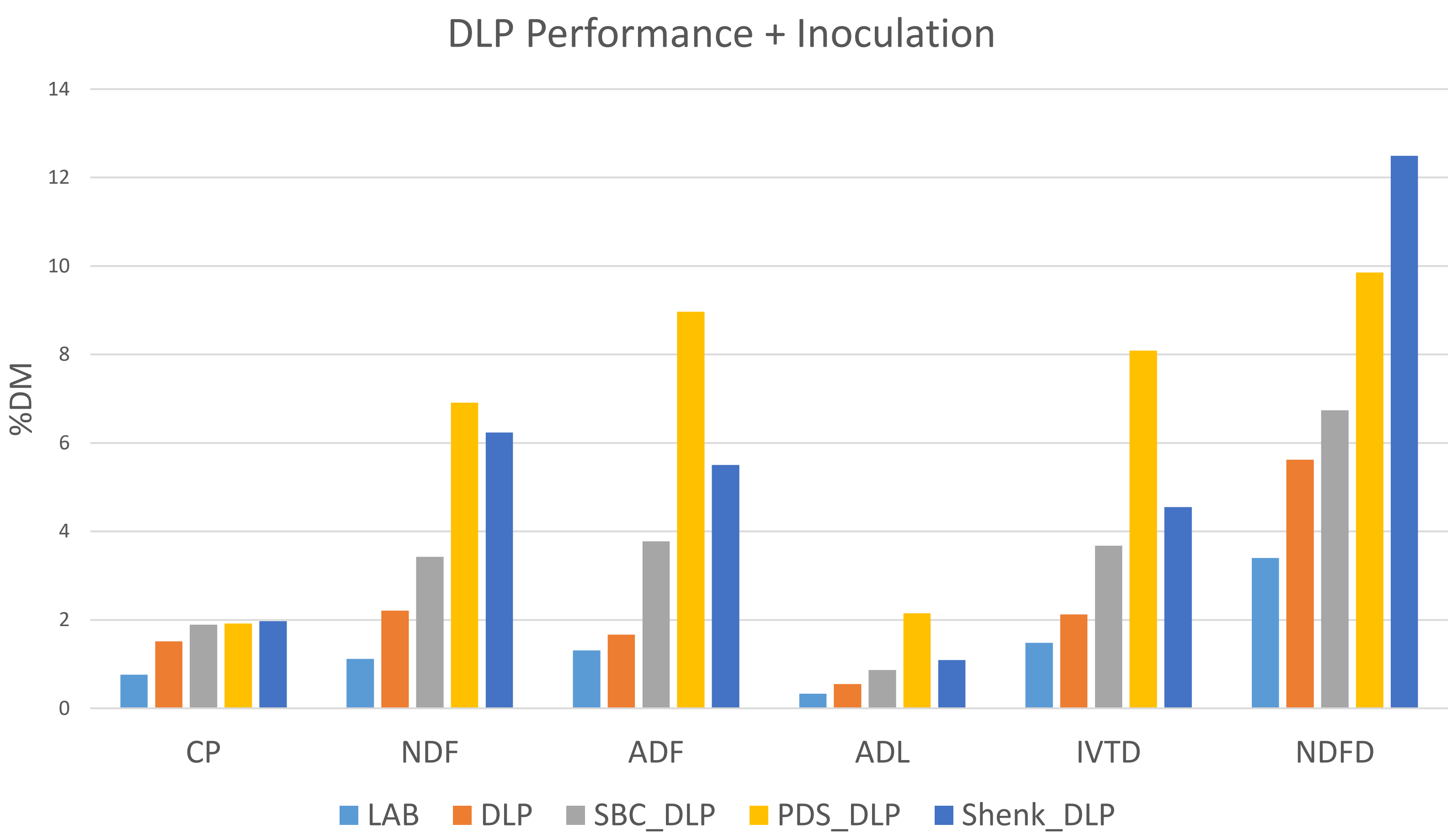
DA SEPs Alfalfa + Inoculation

SBC (-5%) < S&W (+60%) <PDS (+75%)



DLP SEPs Alfalfa + Inoculation

SBC (+50%) < S&W (+132%) <PDS (+175%)



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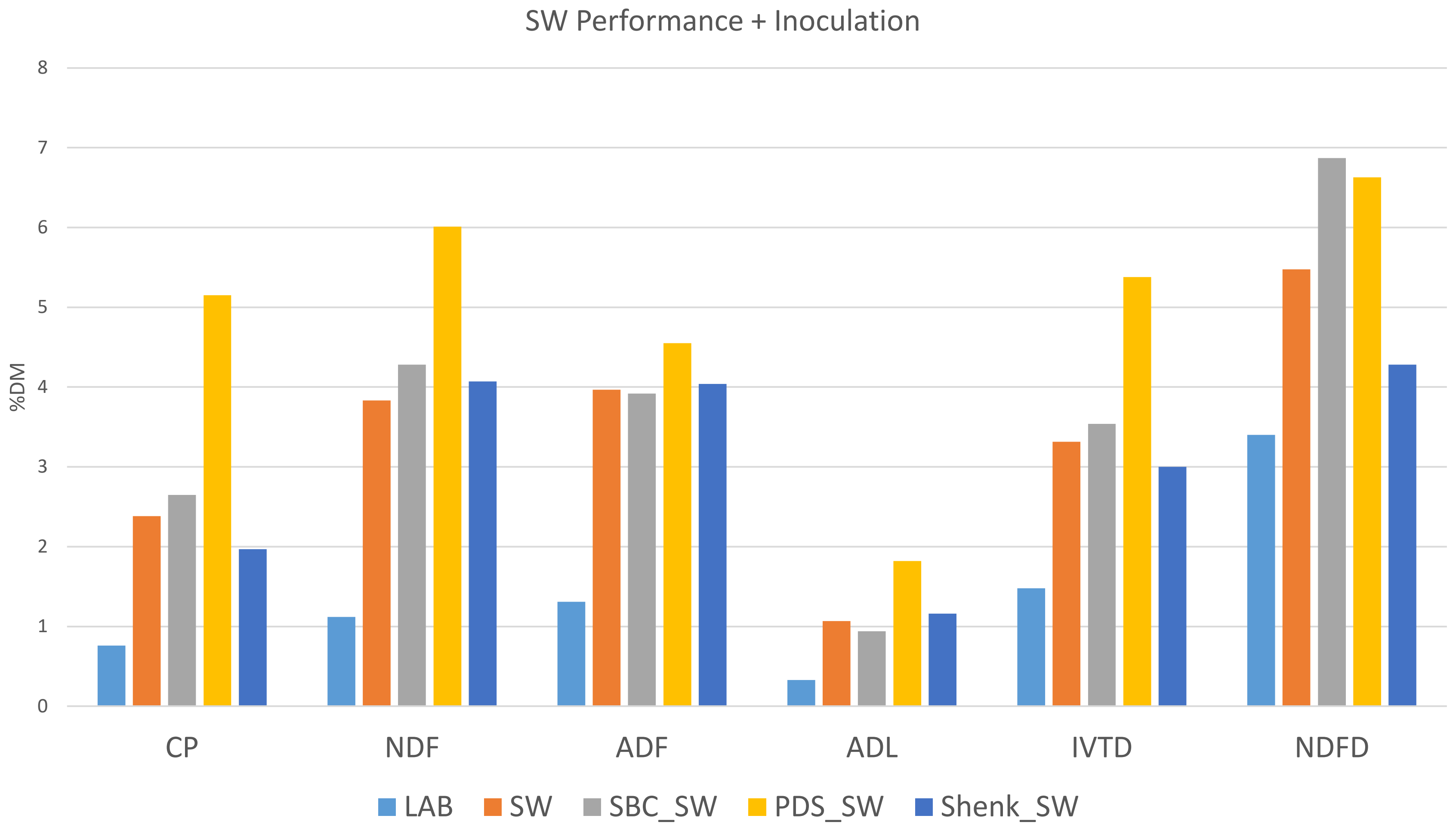
SW SEPs Alfalfa + Inoculation

SBC (+11%) < S&W (+90%) <PDS (+147%)



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Conclusions

Must use many bullets to kill the beast

- Spectra correction: sometime the most sophisticated method is not the best choice
- Inoculation: highly effective, always have this options included
- Reduce calibration sensistivity (fewer PLS component, orthogonalization, REP file….)
- Bias adjustment of results may at the end be necessary

Conclusions

- Clearly one method would not fit all possible sensors
- Must have a high degree in chemometric to evaluate all possible solutions

looking for the future:

  - Easier and more effective methods of spectra transfer (Chemometric for Paolo)
  - May be an intelligent system that would make all possible evaluation

Plans for the Future

learn from mistakes

strive for improvements…

….to make cows and farmers happy

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