

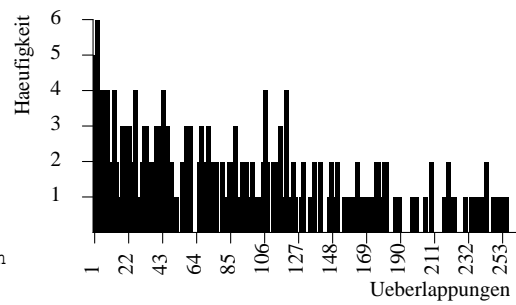
7.4 Matrixdarstellungen

7.4.1 NIR, Standardmethode

```

SV00_MFix.eps
Check Average Spectra
Constant conf. level : Fixed algorithm, Single Sphere Method

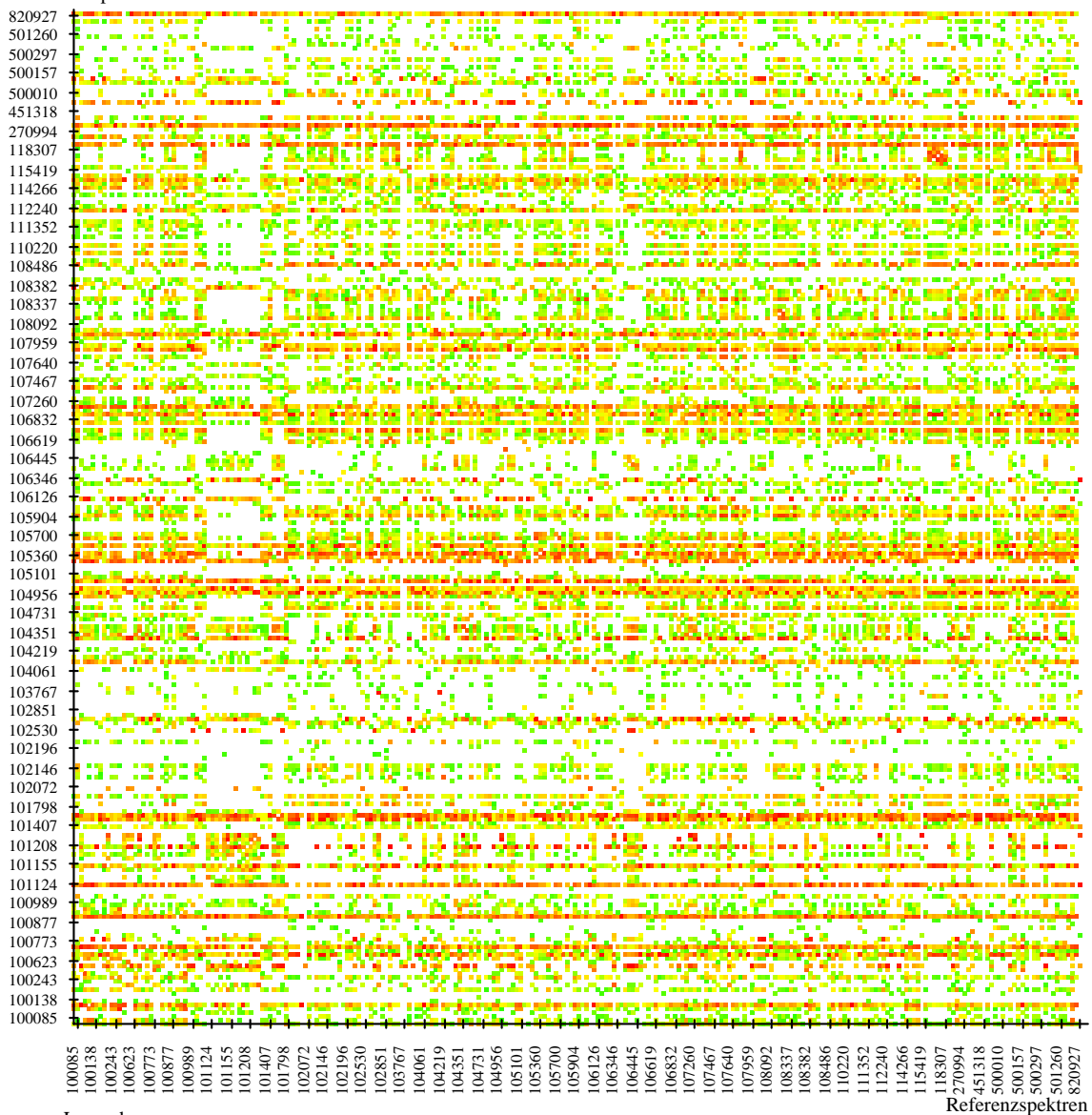
Algorithm:                               Standard
No. of used factor sp.:                   -
Vector normalized spectra:                 Nein
No. of Spectra:                           263
From:                                       3999.71
to:                                         11999.1
Order of Internal Derivation:              0
Smoothing Points for Internal Derivation:  1
    
```



Ueberlapp. Ges.: 23116 (33.55 % bei 1257 (97.7 %) Spektren
 Ueberlapp. Max.:255 bei 1 Spektren

wahr positiv: 45790 falsch negativ: 23116 Sensitivitaet: 66.453 %

Getestete Spektren



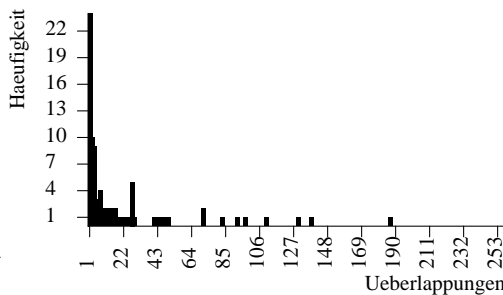
Legende:
 Relative Spektrale Distanz

0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

Abb. N1: Standardmethode ohne Vorbehandlung.

SNV00_MFix.eps
 Check Average Spectra
 Constant conf. level : Fixed algorithm, Single Sphere Method

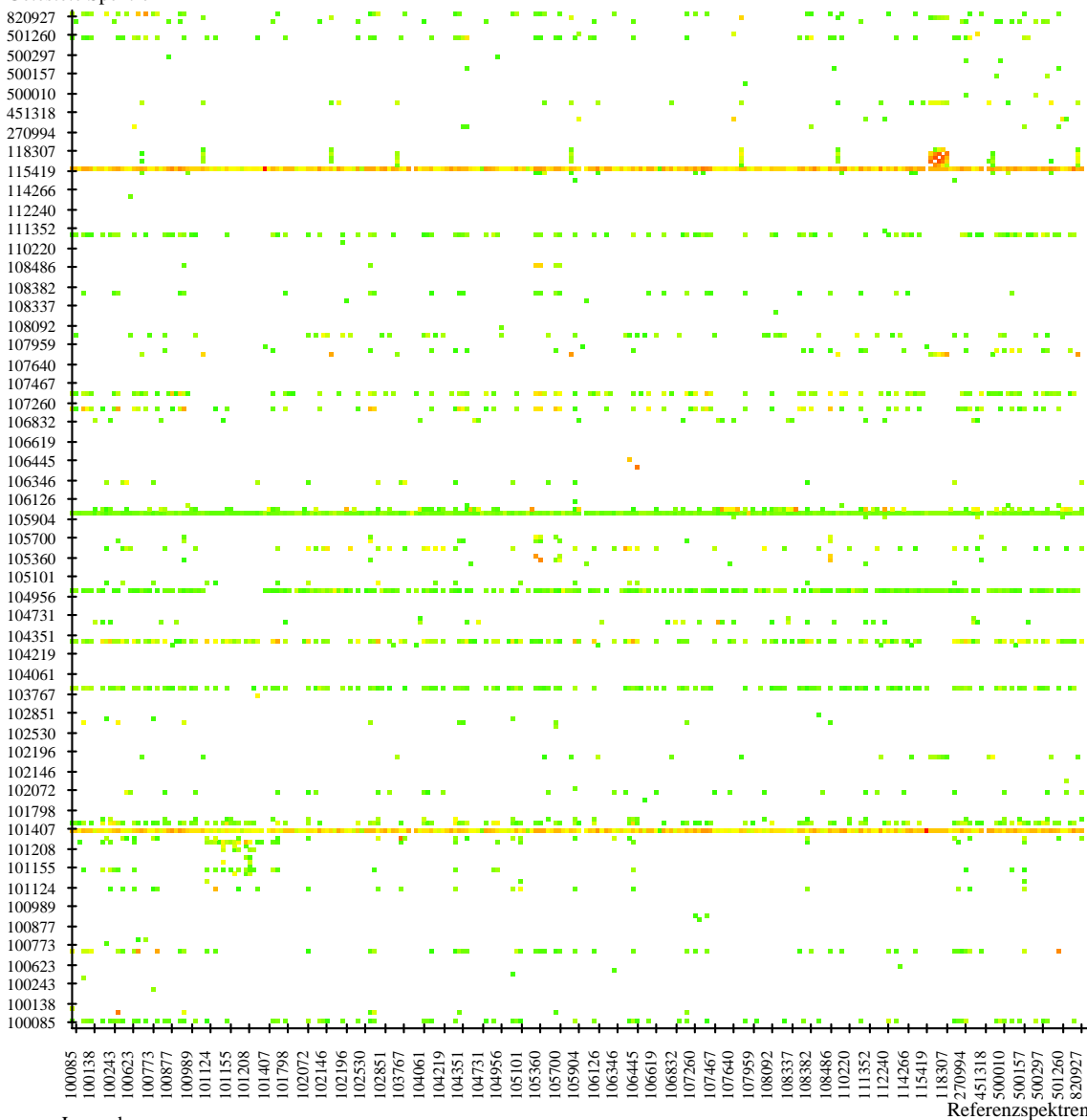
Algorithm: Standard
 No. of used factor sp.: -
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 3999.71
 to: 11999.1
 Order of Internal Derivation: 0
 Smoothing Points for Internal Derivation: 1



Ueberlapp. Ges.: 2565 (3.72 %) bei 97 (36.8 %) Spektren
 Ueberlapp. Max.: 260 bei 1 Spektren

wahr positiv: 66341 falsch negativ: 2565 Sensitivitaet: 96.278 %

Getestete Spektren



Legende:
 Relative Spektrale Distanz

0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

Abb. N2: Standardmethode (Vektornormierung).

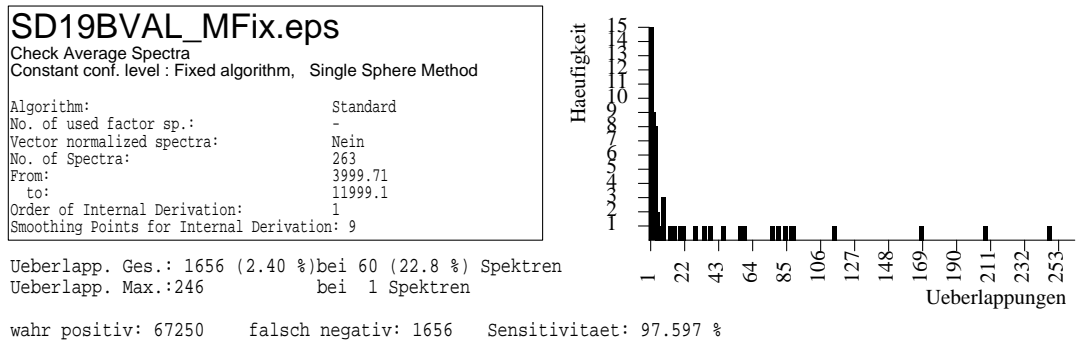


Abb. N3: Standardmethode (1. Ableitung).

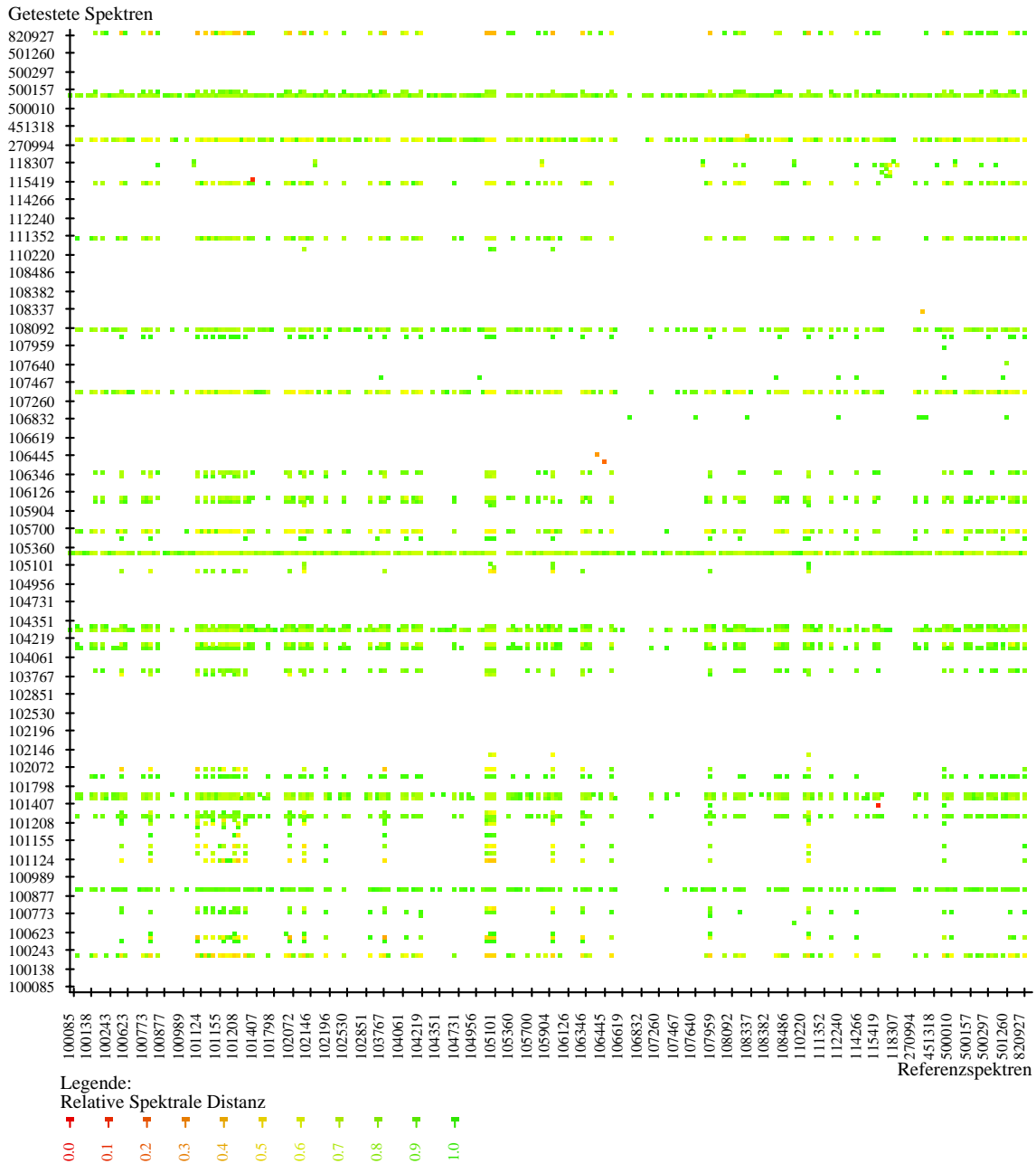
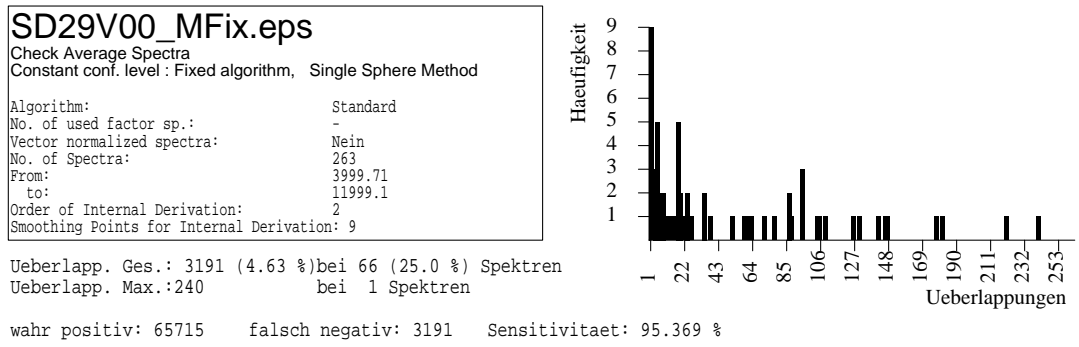


Abb. N4: Standardmethode (2. Ableitung).

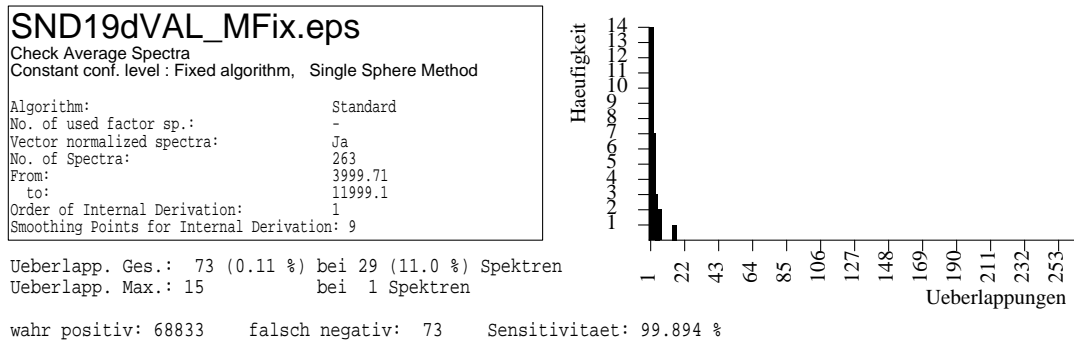
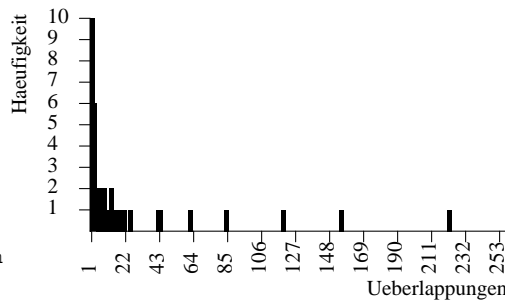


Abb. N5: Standardmethode (Vektornormierung und 1. Ableitung).

SND29V00_MFix.eps
 Check Average Spectra
 Constant conf. level : Fixed algorithm, Single Sphere Method

Algorithm: Standard
 No. of used factor sp.: -
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 3999.71
 to: 11999.1
 Order of Internal Derivation: 2
 Smoothing Points for Internal Derivation: 9



Ueberlapp. Ges.: 2769 (4.02 %) bei 48 (18.2 %) Spektren
 Ueberlapp. Max.: 260 bei 7 Spektren

wahr positiv: 66137 falsch negativ: 2769 Sensitivitaet: 95.981 %

Getestete Spektren



Legende:
 Relative Spektrale Distanz

0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

Abb. N6: Standardmethode (Vektornormierung und 2. Ableitung).

7.4.2 NIR, Faktormethode

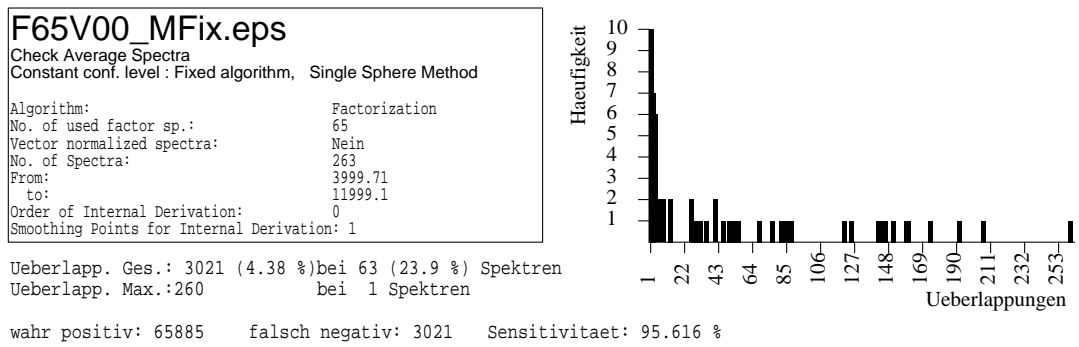
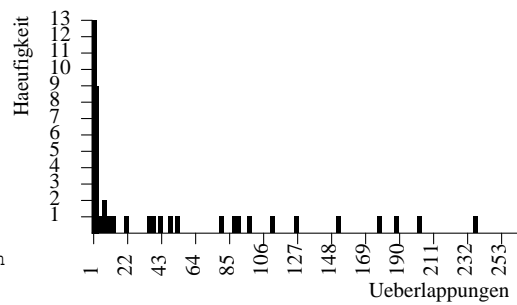


Abb. N7: Faktormethode (65 Faktoren).

F65NV00_MFix.eps
 Check Average Spectra
 Constant conf. level: Fixed algorithm, Single Sphere Method

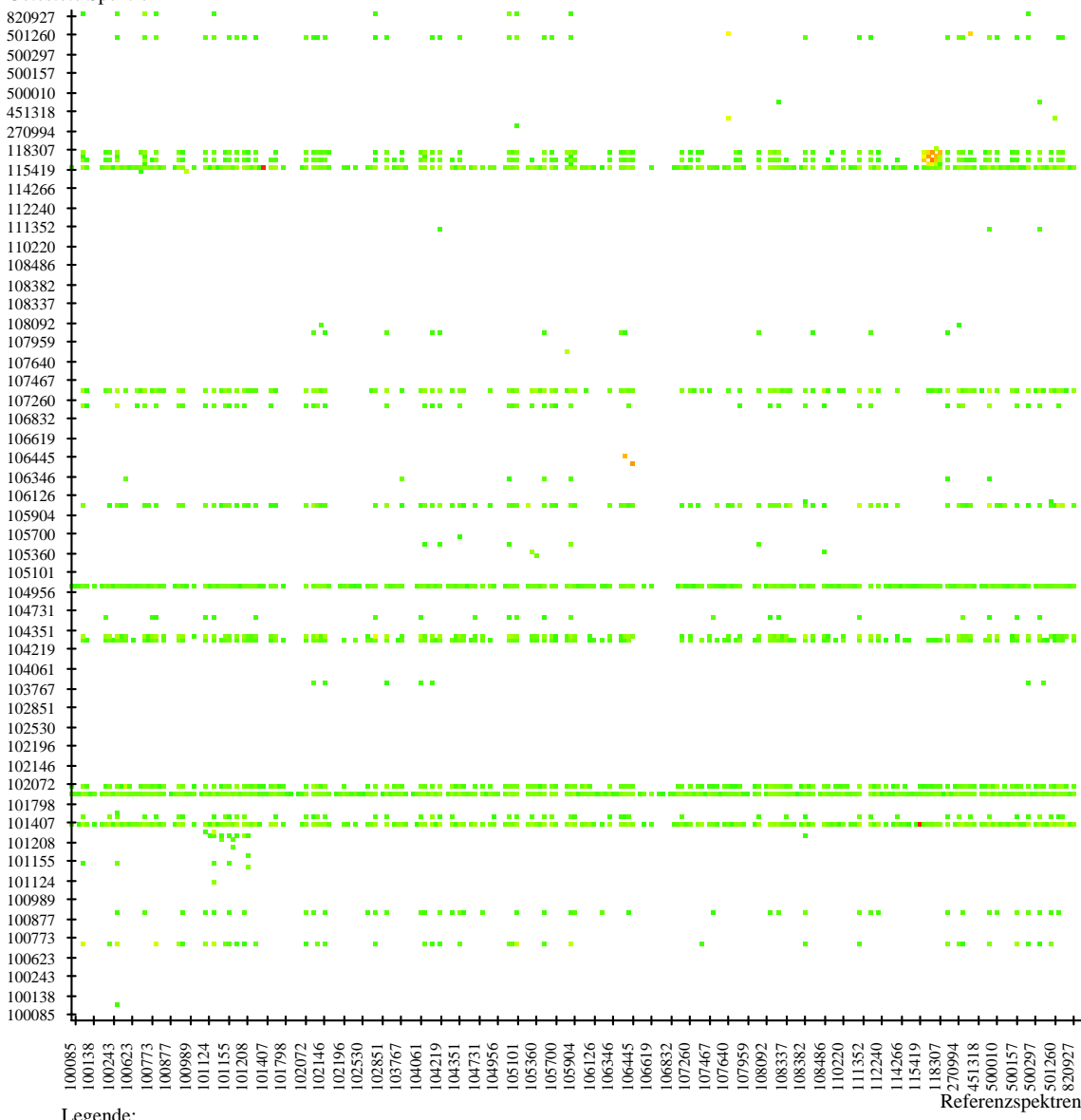
Algorithm: Factorization
 No. of used factor sp.: 65
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 3999.71
 to: 11999.1
 Order of Internal Derivation: 0
 Smoothing Points for Internal Derivation: 1



Ueberlapp. Ges.: 1883 (2.73 %) bei 50 (19.0 %) Spektren
 Ueberlapp. Max.: 236 bei 1 Spektren

wahr positiv: 67023 falsch negativ: 1883 Sensitivitaet: 97.267 %

Getestete Spektren



Legende:
 Relative Spektrale Distanz

0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

Abb. N8: Faktormethode (65 Faktoren, Vektornormierung).

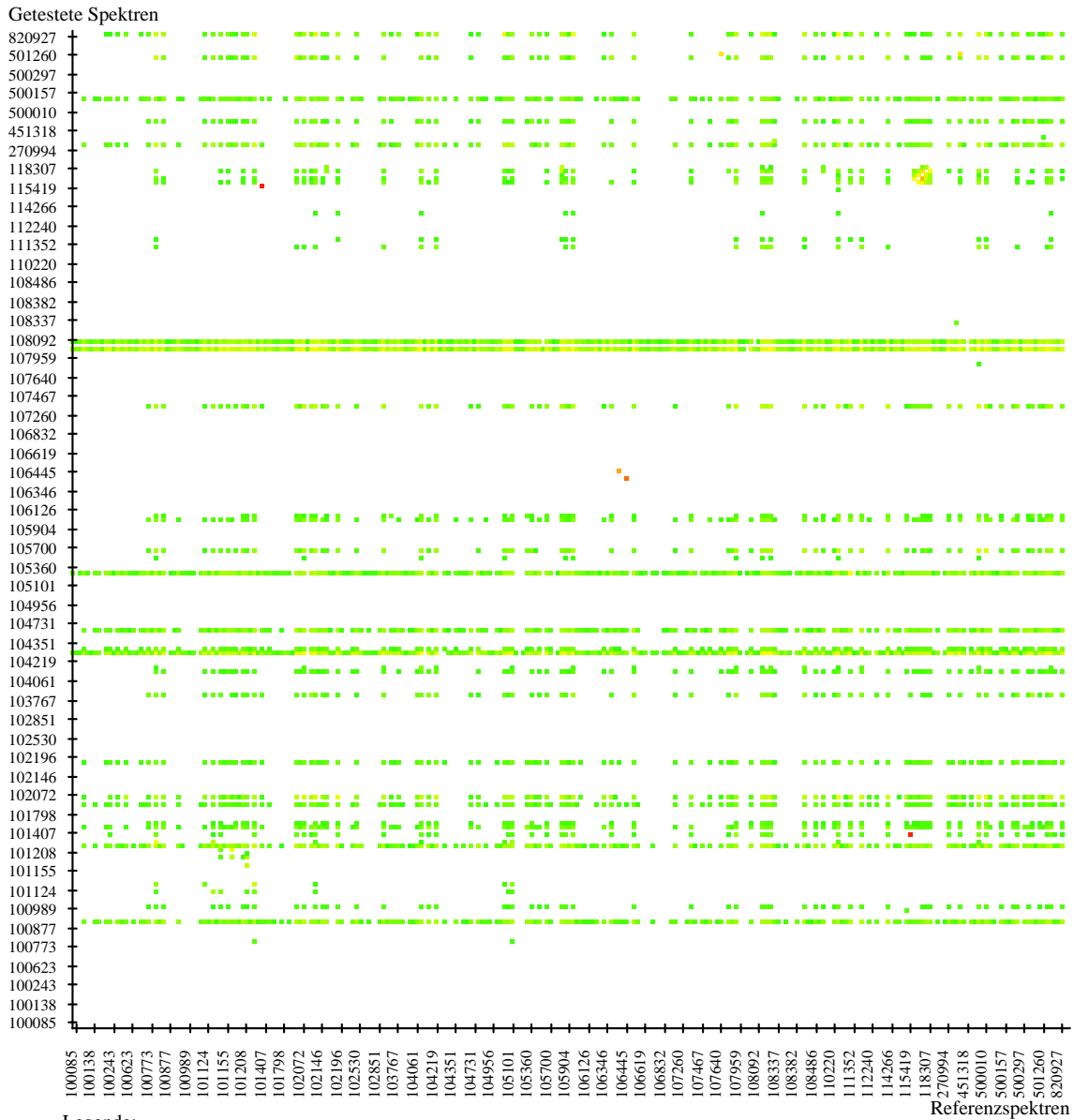
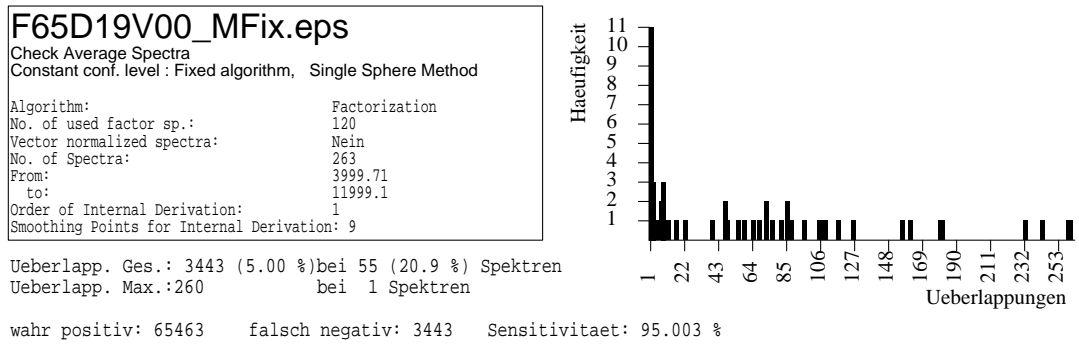


Abb. N9: Faktormethode (65 Faktoren, 1. Ableitung).

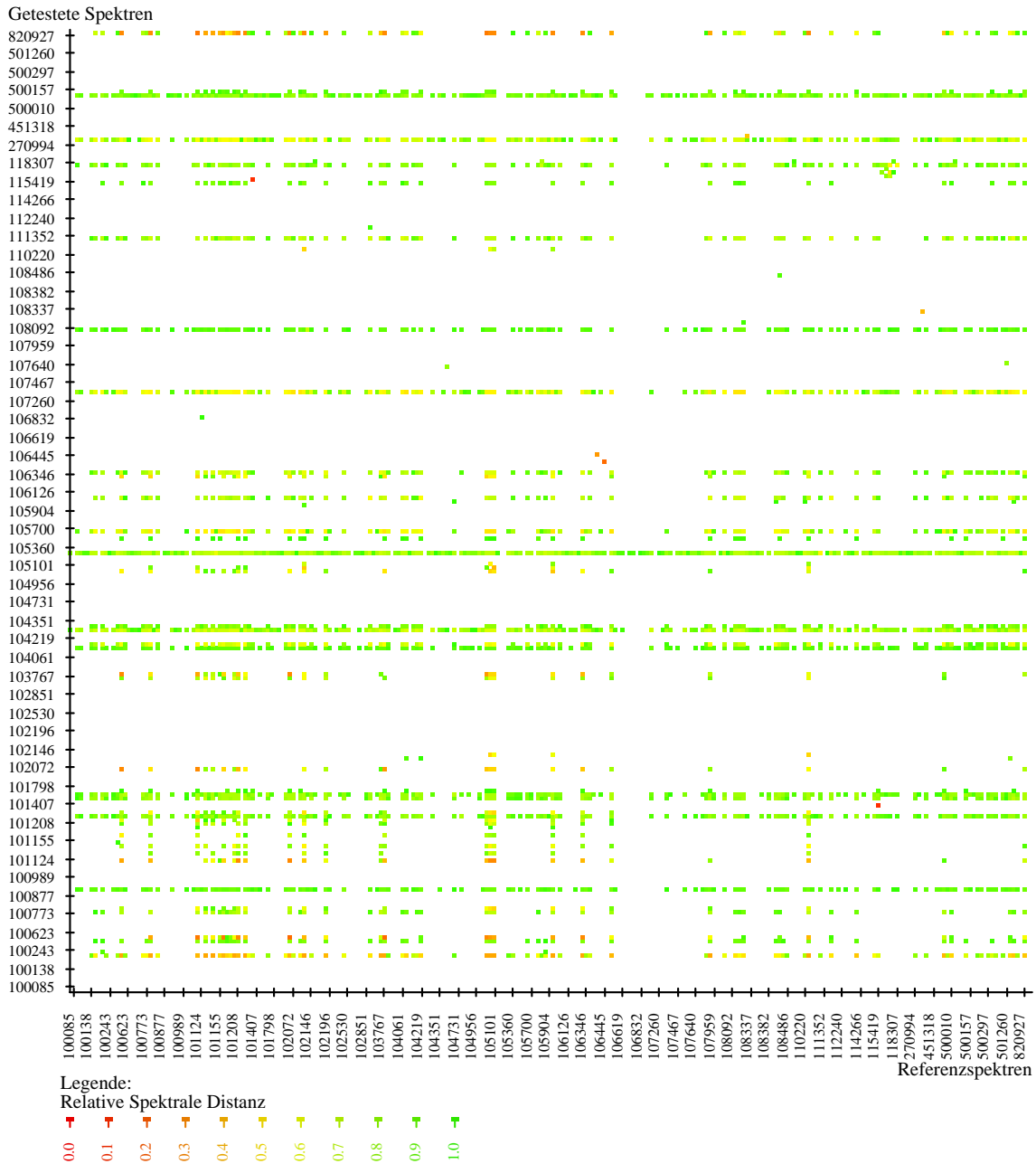
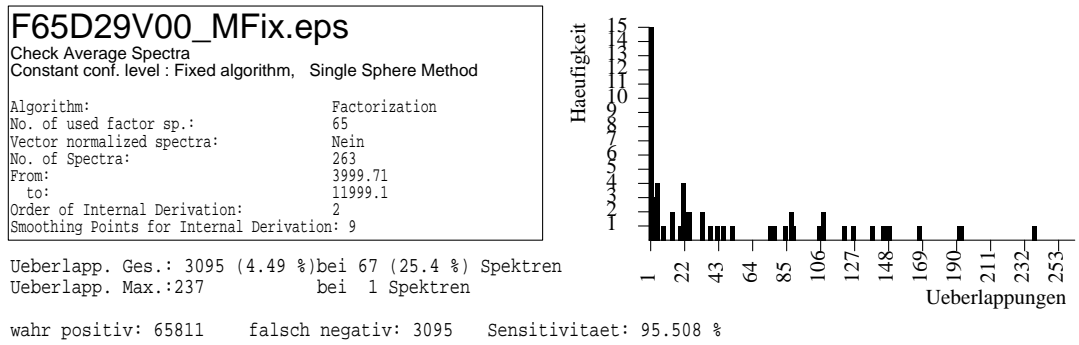
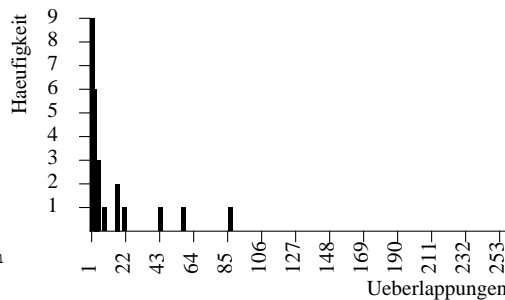


Abb. N10: Faktormethode (65 Faktoren, 2. Ableitung).

F65ND19V00_MFix.eps
 Check Average Spectra
 Constant conf. level: Fixed algorithm, Single Sphere Method

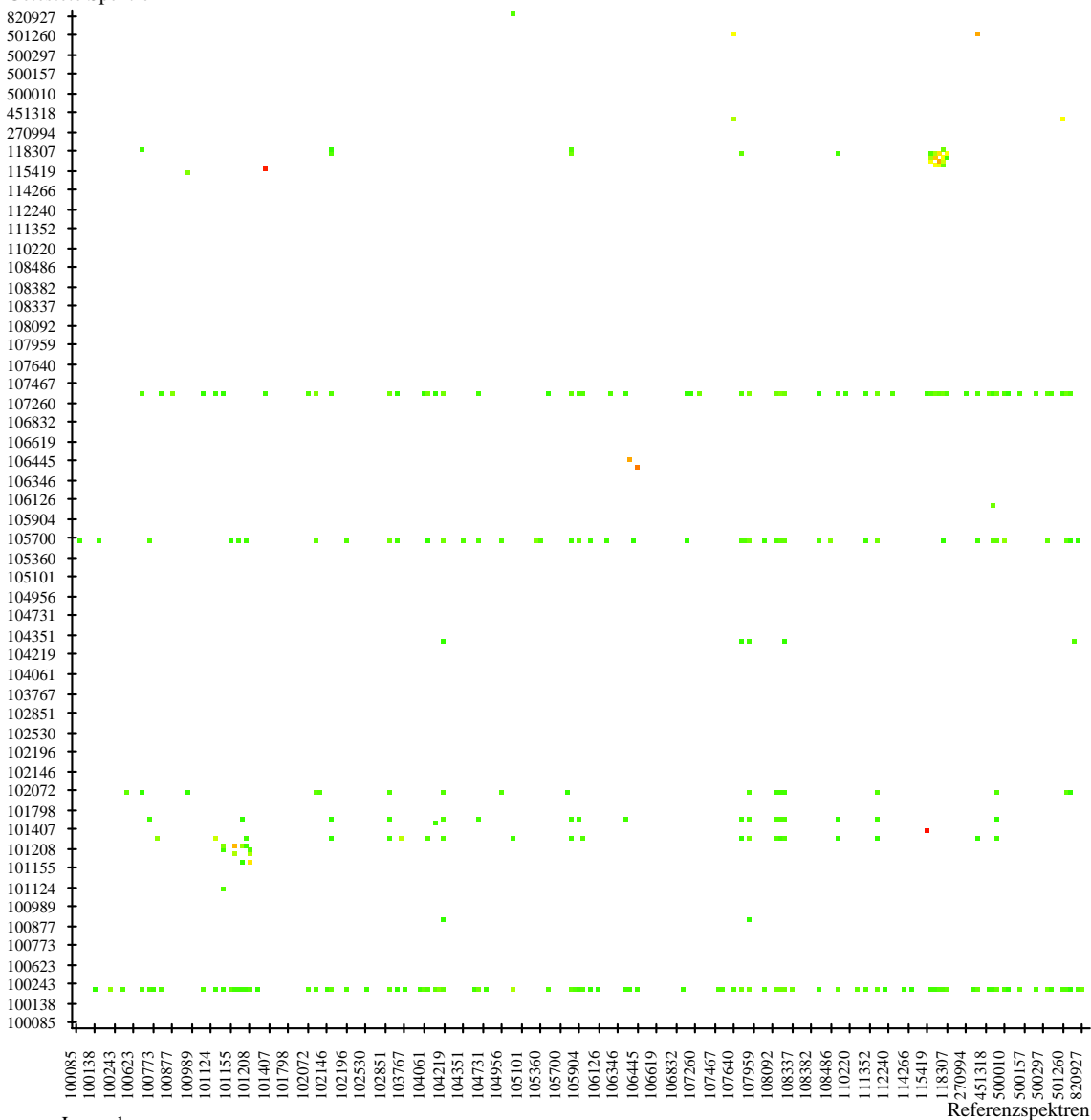
Algorithm: Factorization
 No. of used factor sp.: 65
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 3999.71
 to: 11999.1
 Order of Internal Derivation: 1
 Smoothing Points for Internal Derivation: 9



Ueberlapp. Ges.: 292 (0.42 %) bei 28 (10.6 %) Spektren
 Ueberlapp. Max.: 86 bei 1 Spektren

wahr positiv: 68614 falsch negativ: 292 Sensitivitaet: 99.576 %

Getestete Spektren



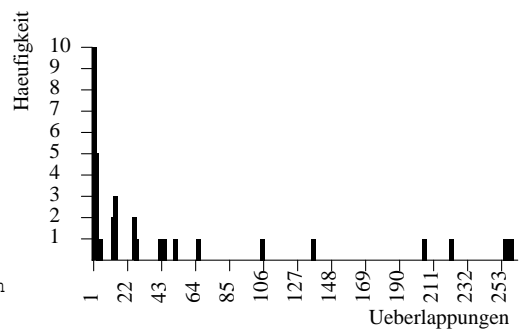
Legende:
 Relative Spektrale Distanz

0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

Abb. N11: Faktormethode (65 Faktoren, Vektornormierung und 1. Ableitung).

f65nd29val_MFix.eps
 Check Average Spectra
 Constant conf. level: Fixed algorithm, Single Sphere Method

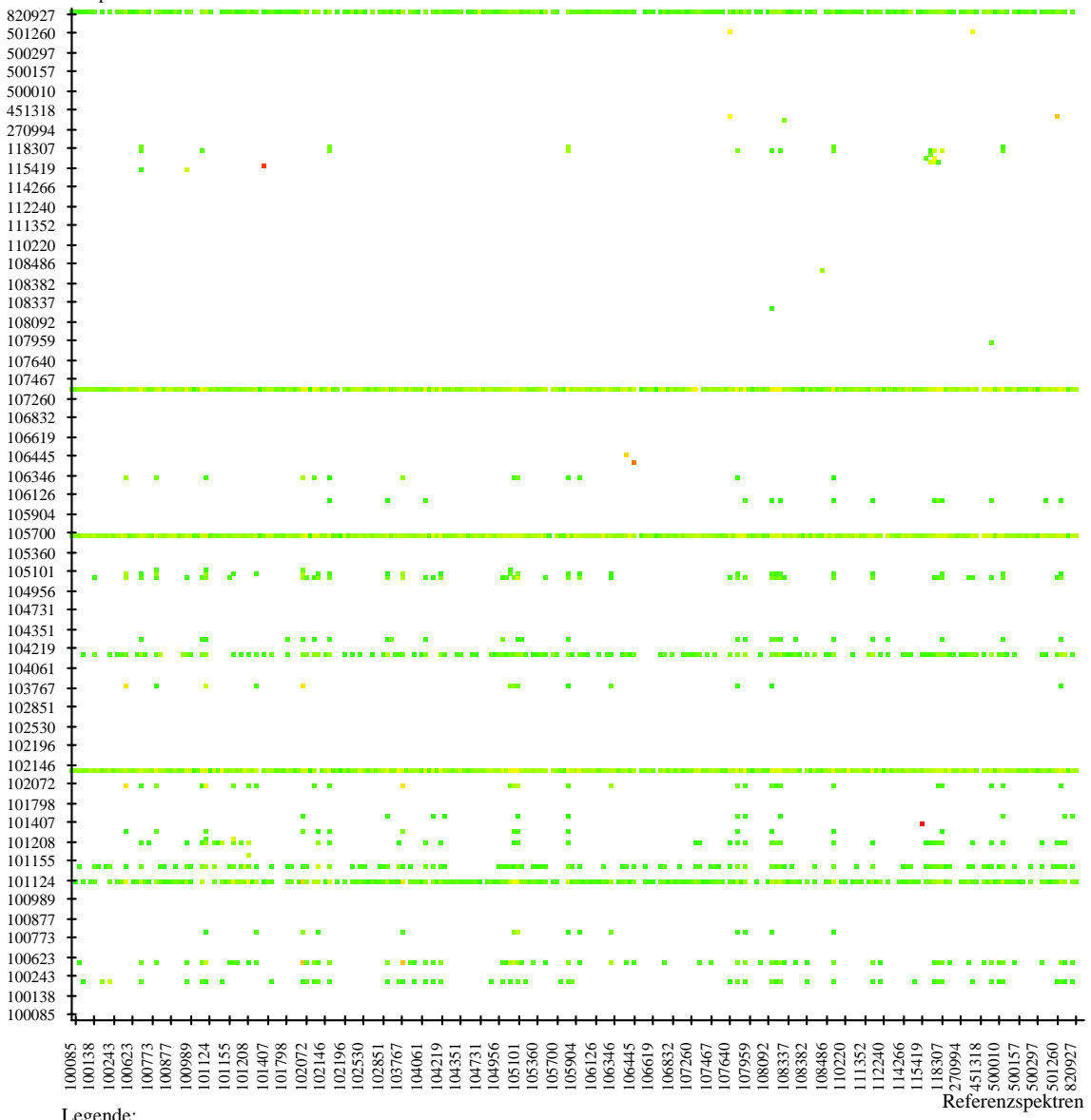
Algorithm: Factorization
 No. of used factor sp.: 65
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 3999.71
 to: 11999.1
 Order of Internal Derivation: 2
 Smoothing Points for Internal Derivation: 9



Ueberlapp. Ges.: 1841 (2.67 %) bei 39 (14.8 %) Spektren
 Ueberlapp. Max.: 258 bei 1 Spektren

wahr positiv: 67065 falsch negativ: 1841 Sensitivitaet: 97.328 %

Getestete Spektren



Legende:
 Relative Spektrale Distanz

0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

Abb. N12: Faktormethode (65 Faktoren, Vektornormierung und 2. Ableitung).

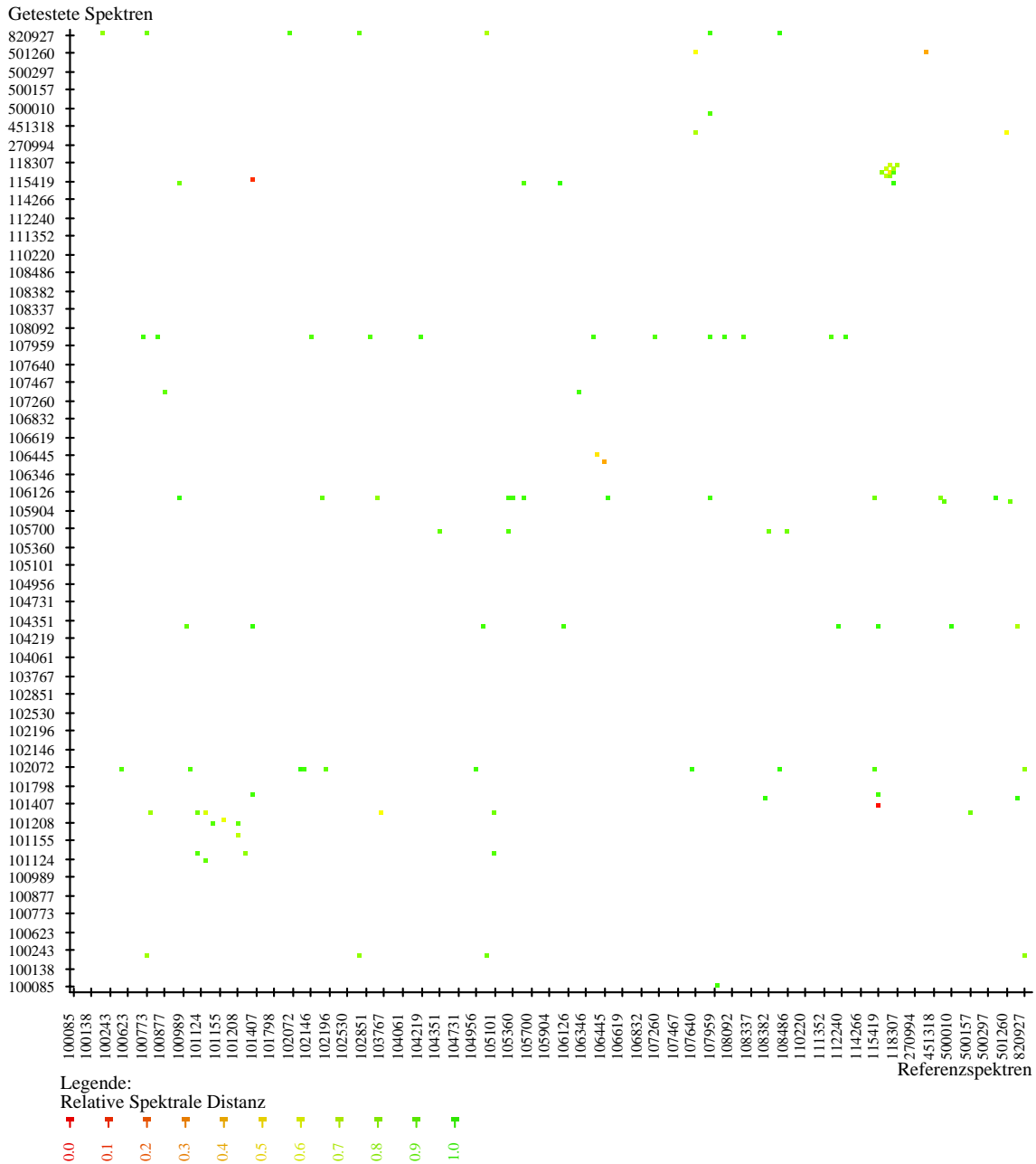
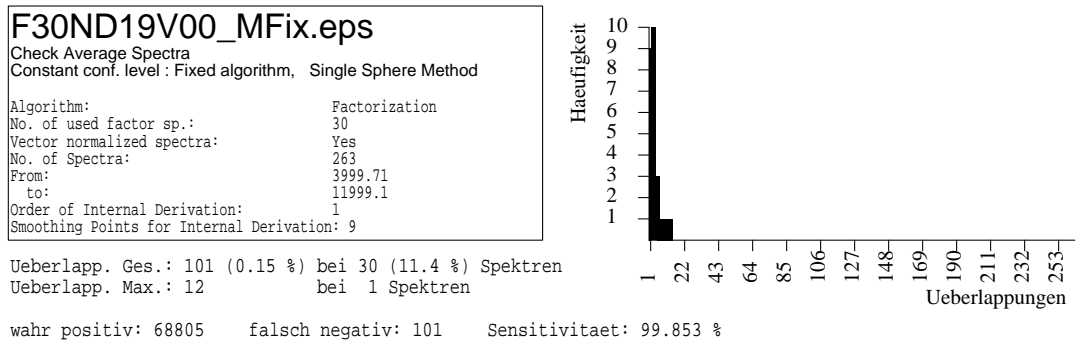


Abb. N13: Faktormethode (30 Faktoren, Vektornormierung und 1. Ableitung).

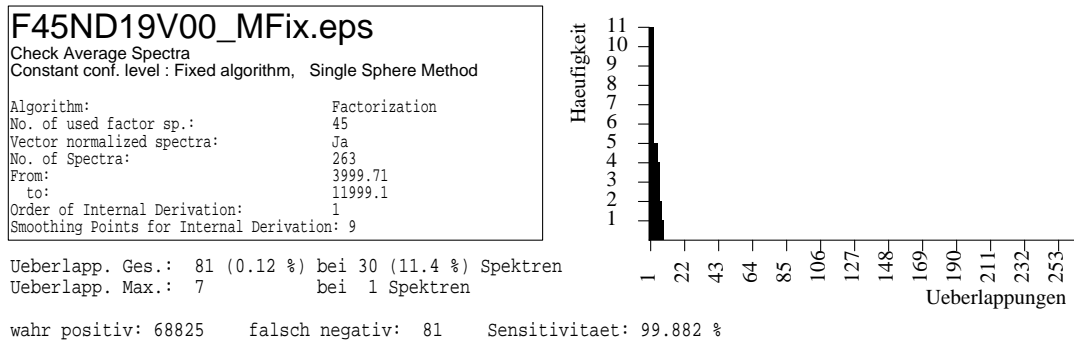


Abb. N14: Faktormethode (45 Faktoren, Vektornormierung und 1. Ableitung).

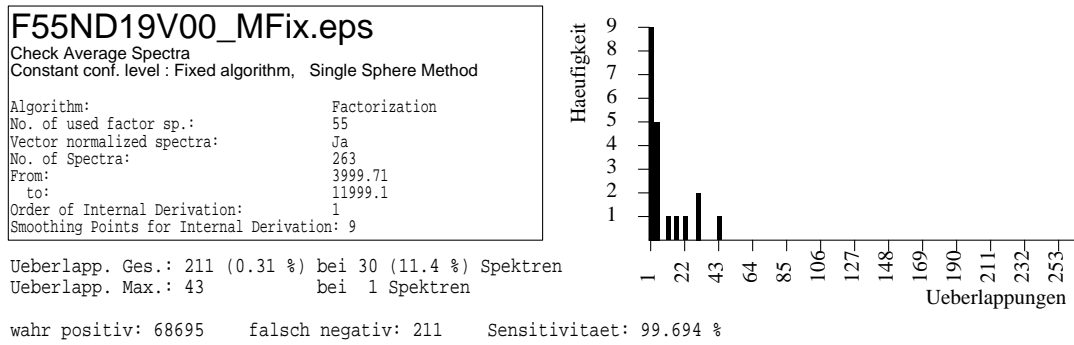


Abb. N15: Faktormethode (55 Faktoren, Vektornormierung und 1. Ableitung).

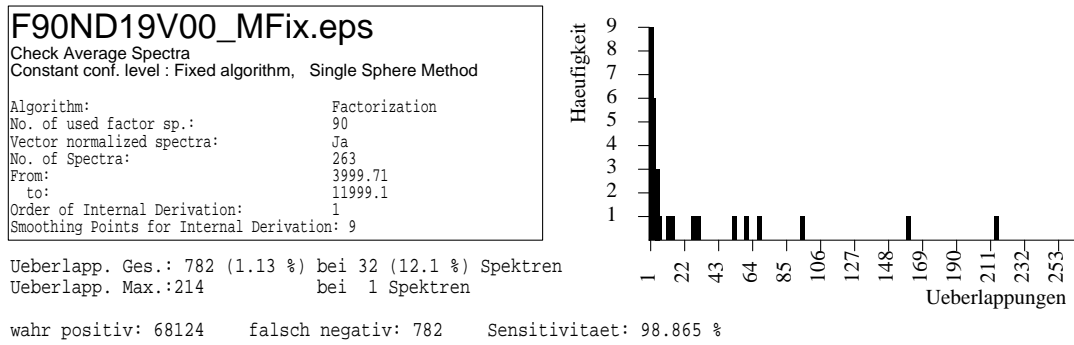


Abb. N16: Faktormethode (90 Faktoren, Vektornormierung und 1. Ableitung).

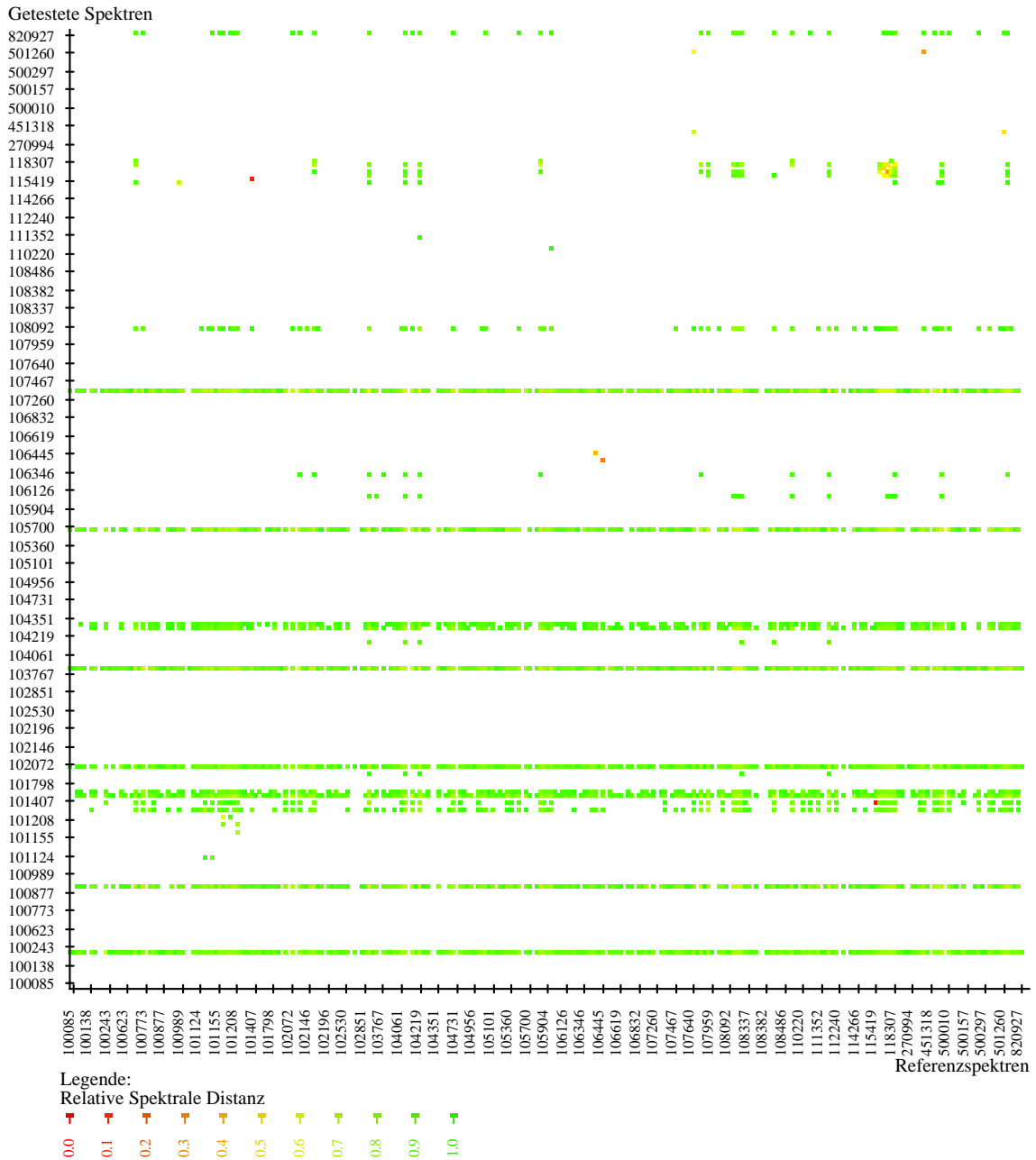
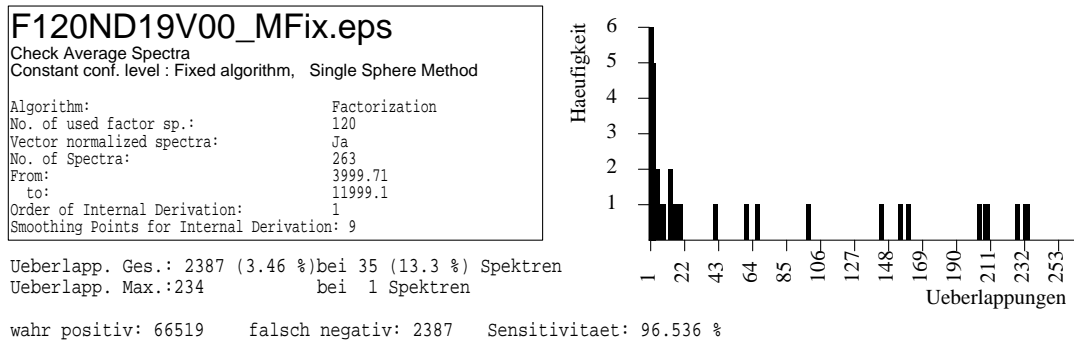


Abb. N17: Faktormethode (120 Faktoren, Vektornormierung und 1. Ableitung).

7.4.3 NIR, Variation des Spektralbereiches

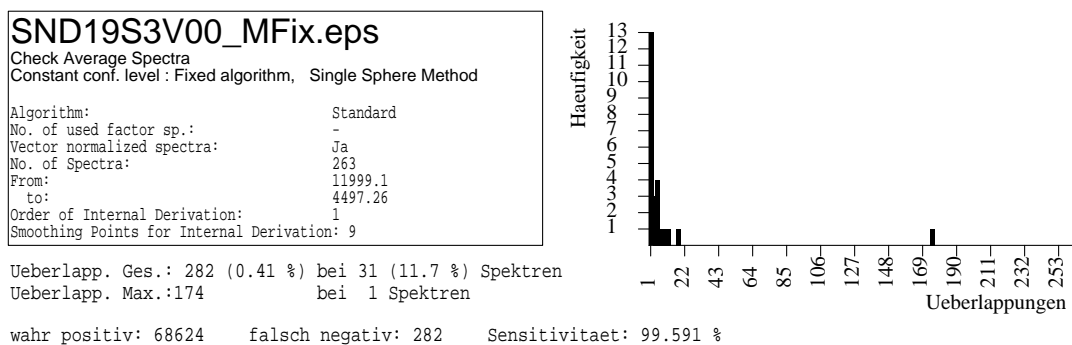


Abb. N18: Standardmethode (Vektornormierung und 1. Ableitung, 12000 cm^{-1} bis 4500 cm^{-1}).

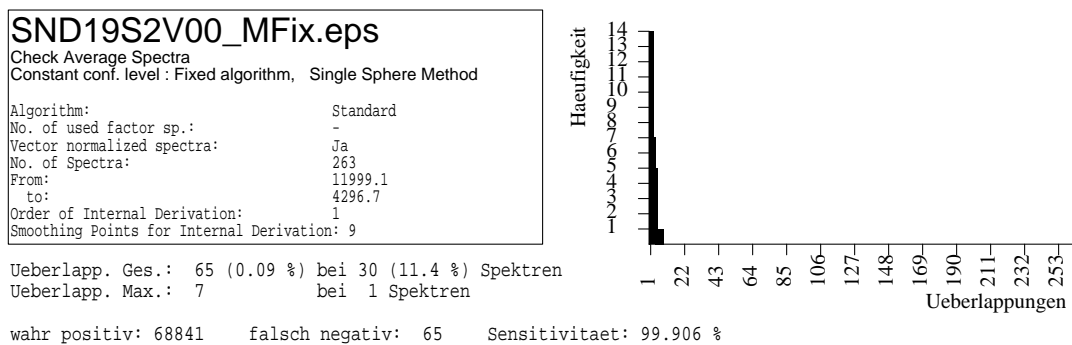


Abb. N19: Standardmethode (Vektornormierung und 1. Ableitung, 12000 cm^{-1} bis 4300 cm^{-1}).

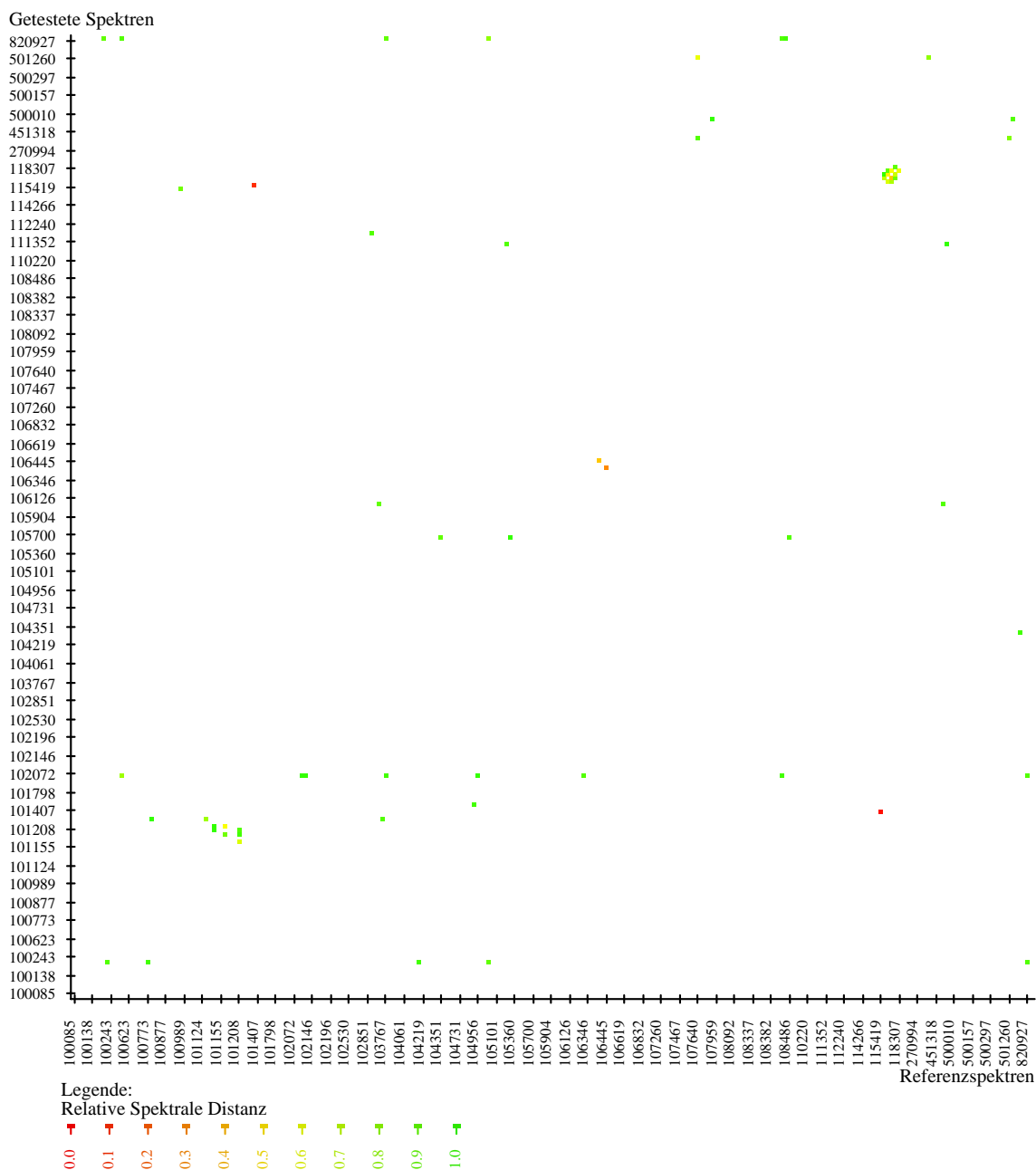
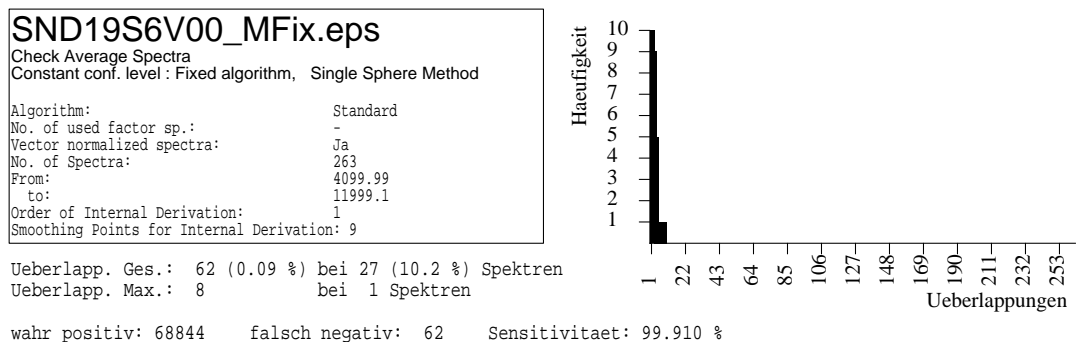
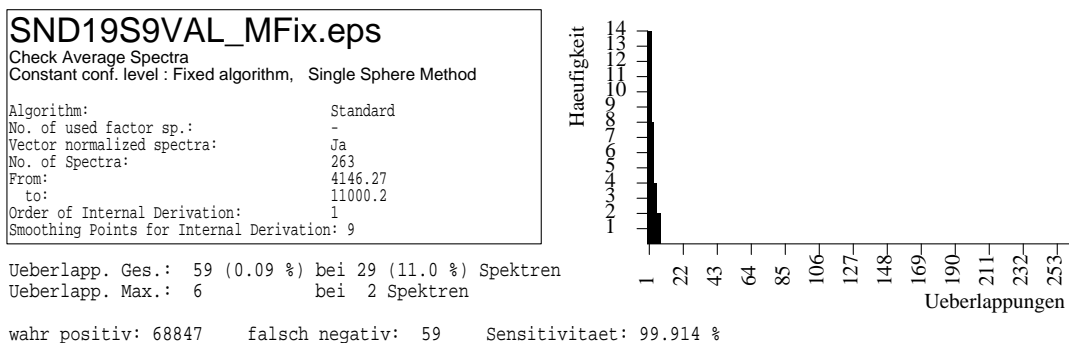


Abb. N20: Standardmethode (Vektornormierung und 1. Ableitung, 12000 cm^{-1} bis 4100 cm^{-1}).



Getestete Spektren

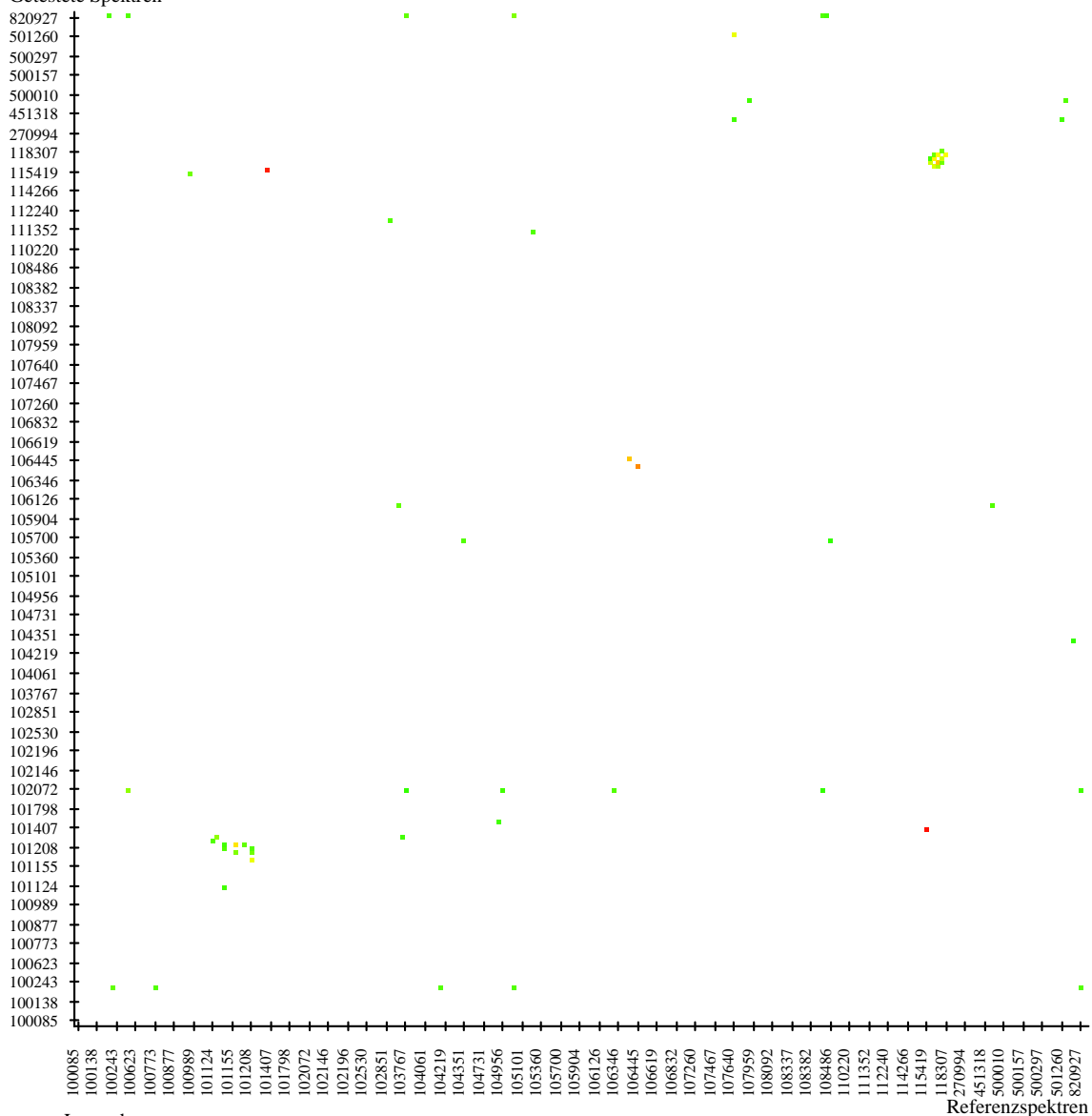


Abb. N21: Standardmethode (Vektornormierung und 1. Ableitung, 11000 cm^{-1} bis 4150 cm^{-1}).

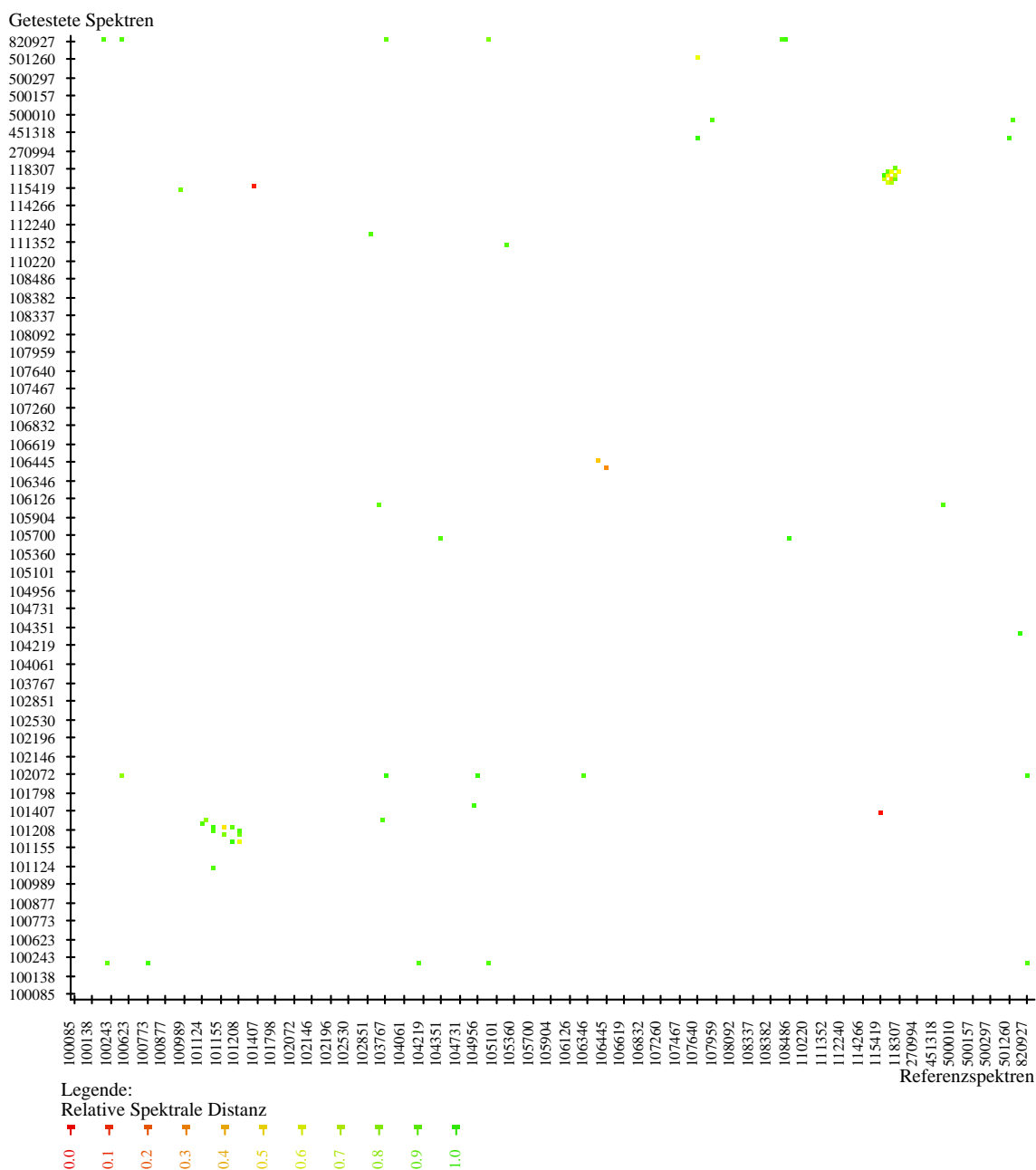
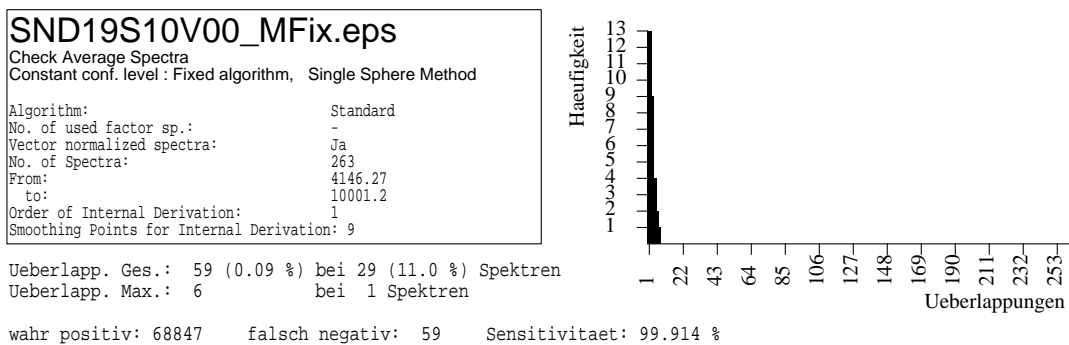


Abb. N22: Standardmethode (Vektornormierung und 1. Ableitung, 10000 cm^{-1} bis 4150 cm^{-1}).

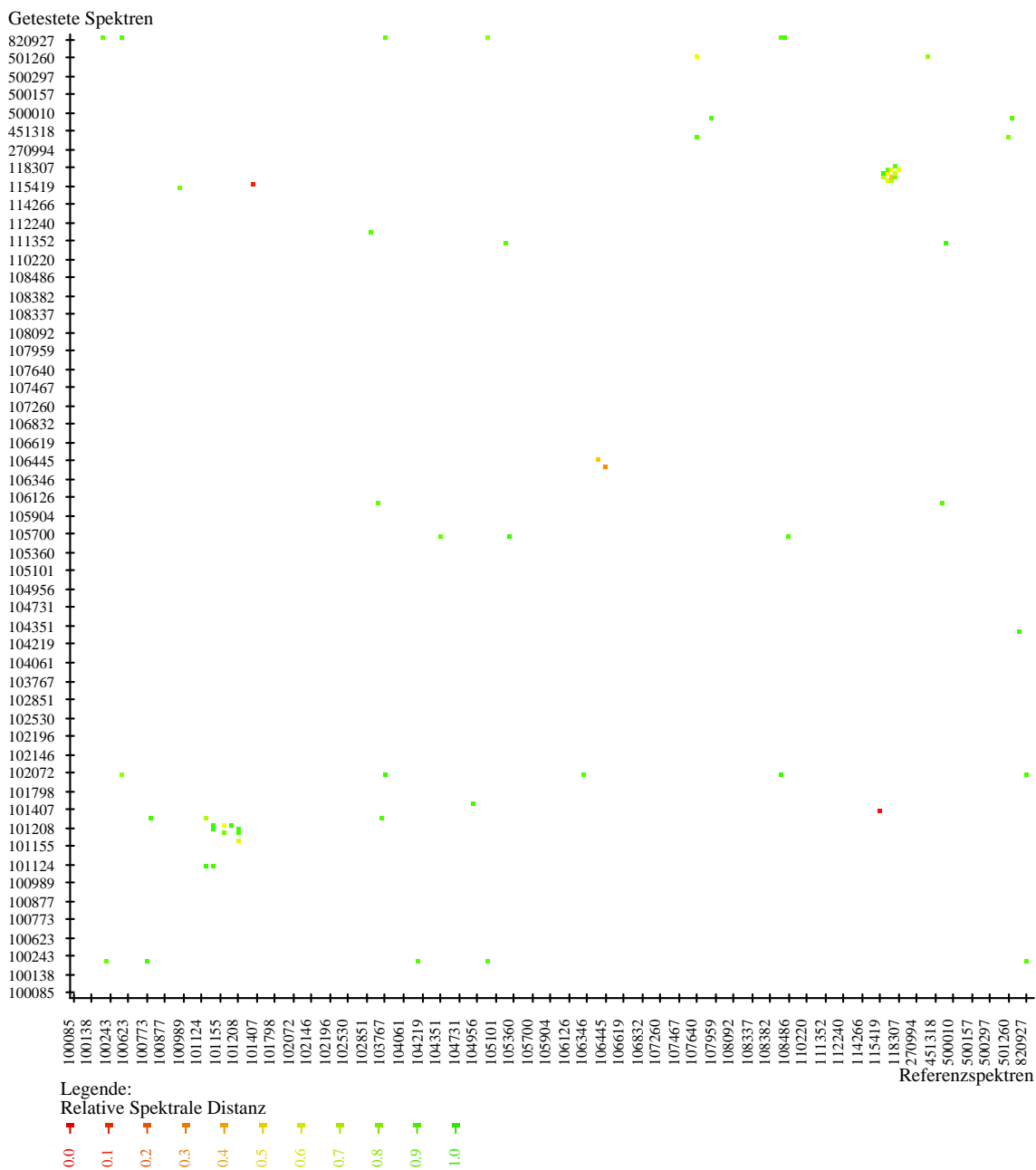
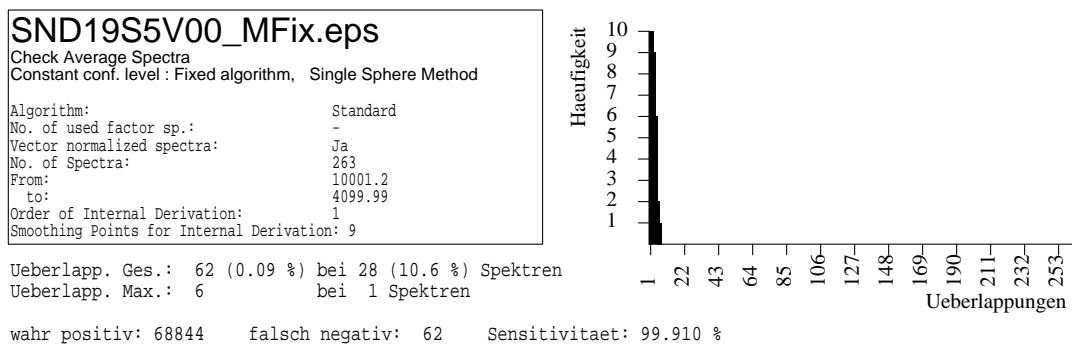


Abb. N23: Standardmethode (Vektornormierung und 1. Ableitung, 10000 cm^{-1} bis 4100 cm^{-1}).

7.4.4 NIR, Variation der Thresholdberechnung

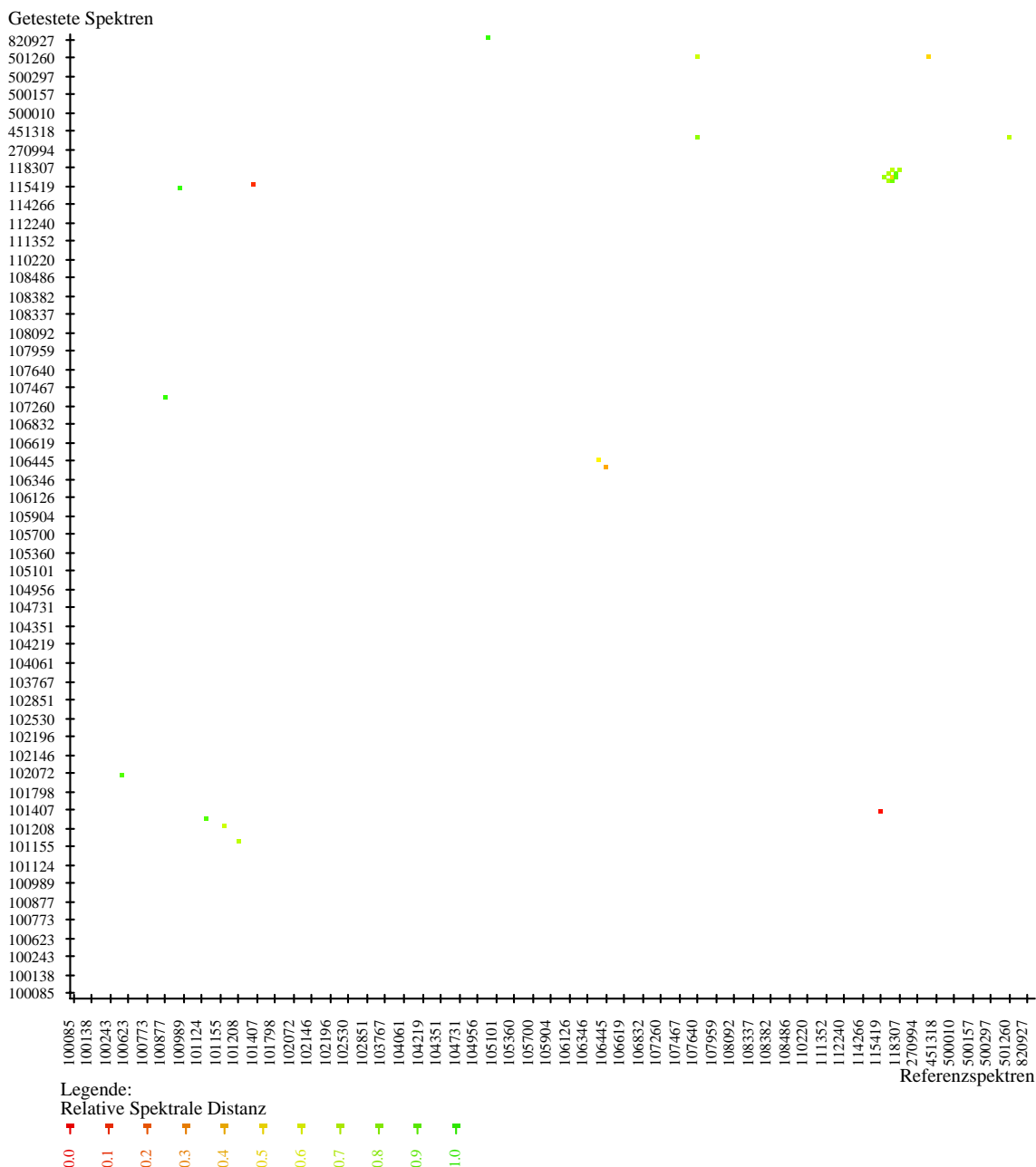
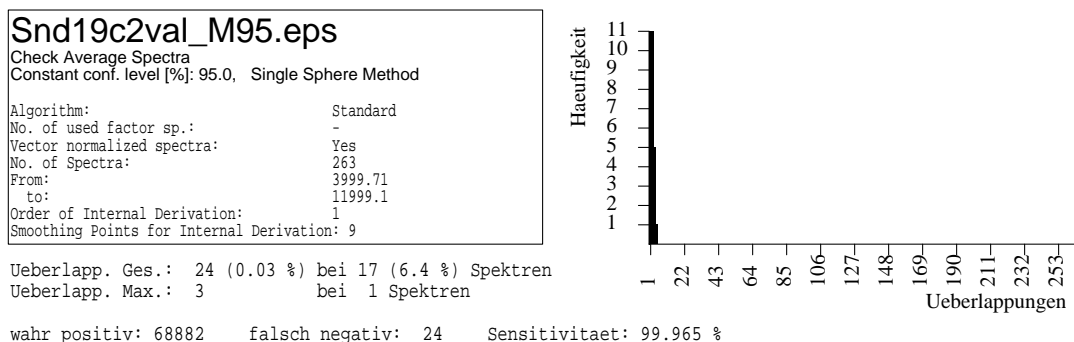


Abb. N24: Standardmethode (Vektornormierung und 1. Ableitung, konstantes Konfidenzniveau von 95 %).

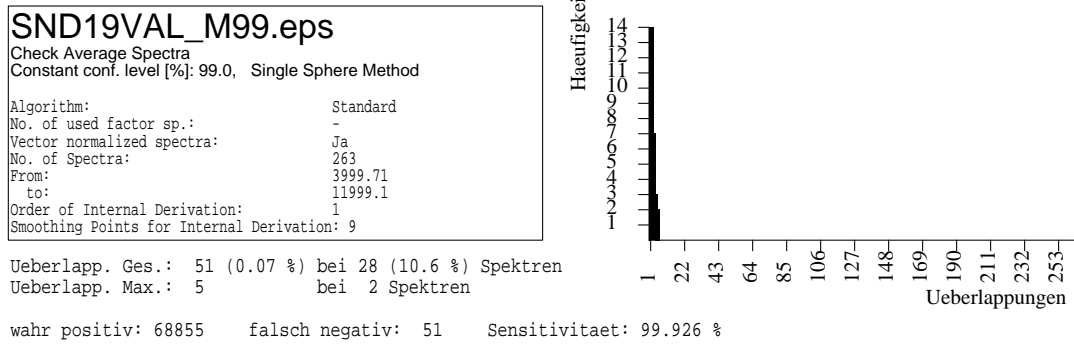
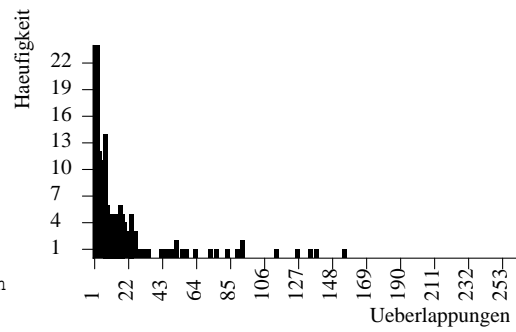


Abb. N25: Standardmethode (Vektornormierung und 1. Ableitung, konstantes Konfidenz-niveau von 99 %).

Snd19v04_MDouble.eps
 Check Average Spectra
 Constant conf. level : Fixed algorithm, Double Sphere Method

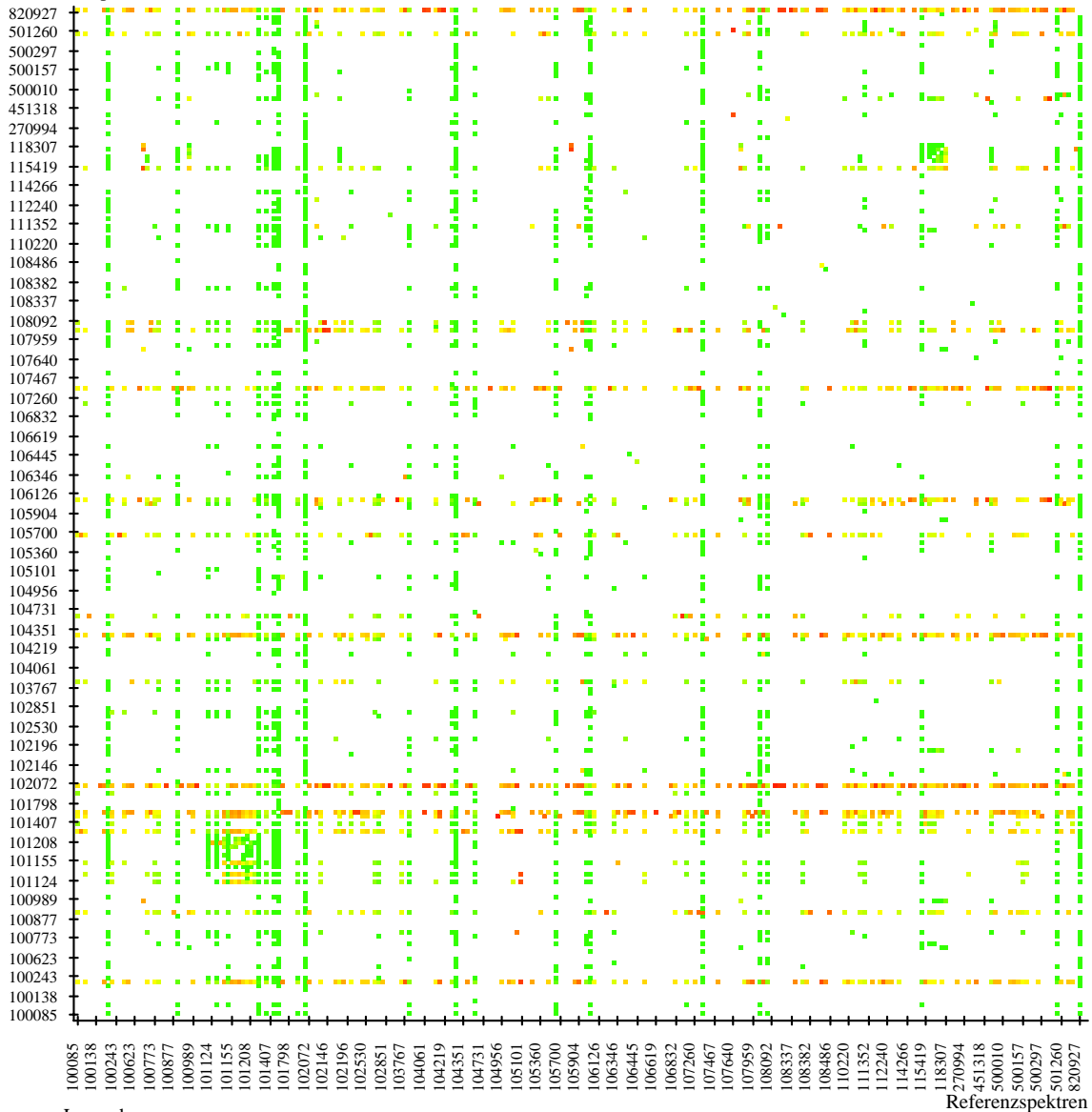
Algorithm: Standard
 No. of used factor sp.: -
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 3999.71
 to: 11999.1
 Order of Internal Derivation: 1
 Smoothing Points for Internal Derivation: 9



Überlapp. Ges.: 3573 (5.19 %) bei 202 (76.8 %) Spektren
 Überlapp. Max.: 155 bei 1 Spektren

wahr positiv: 65333 falsch negativ: 3573 Sensitivitaet: 94.815 %

Getestete Spektren



Legende:
 Relative Spektrale Distanz

0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

Abb. N26: Standardmethode (Vektornormierung und 1. Ableitung, Doppelkugelmodell, Fixed Algorithm).

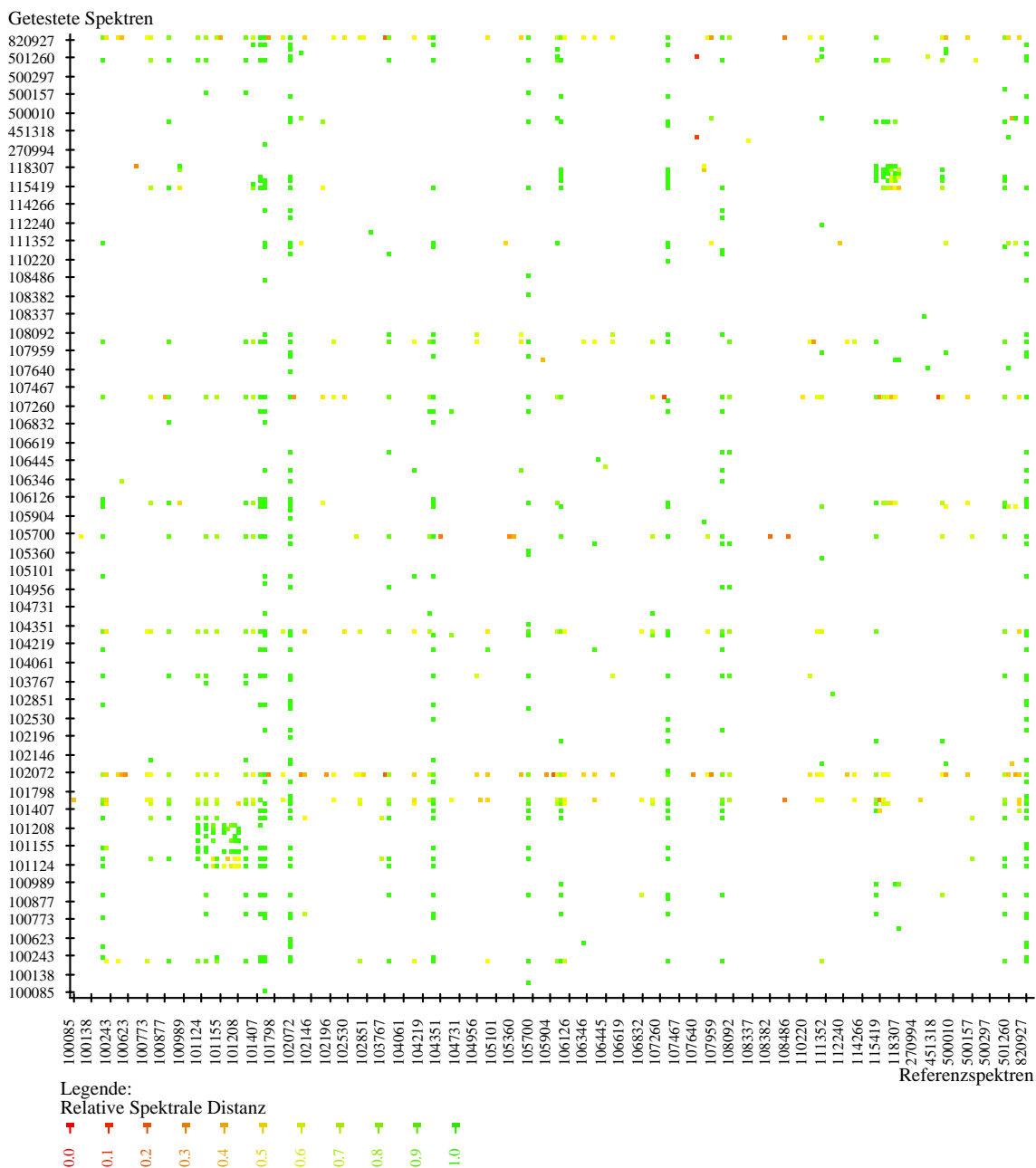
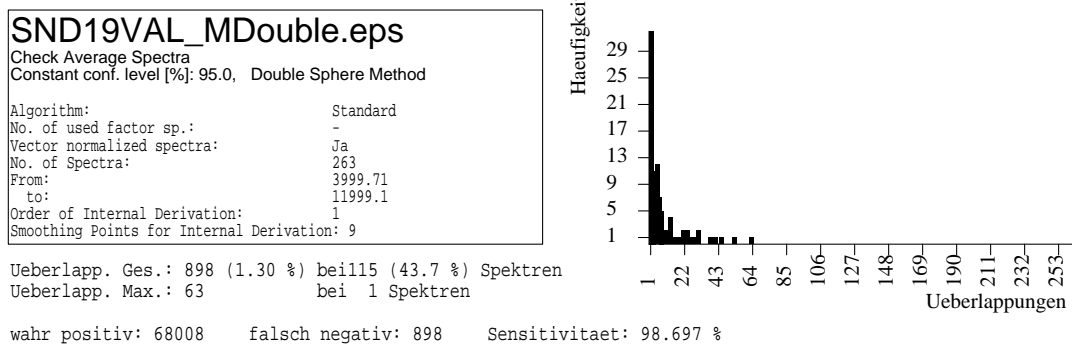
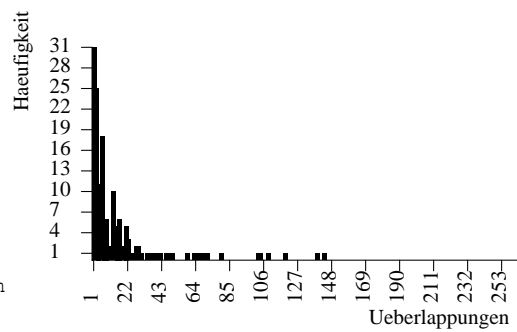


Abb. N27: Standardmethode (Vektornormierung und 1. Ableitung, Doppelkugelmodell, konstantes Konfidenzniveau von 95 %).

SND19bVAL_MDouble.eps
 Check Average Spectra
 Constant conf. level [%]: 99.0, Double Sphere Method

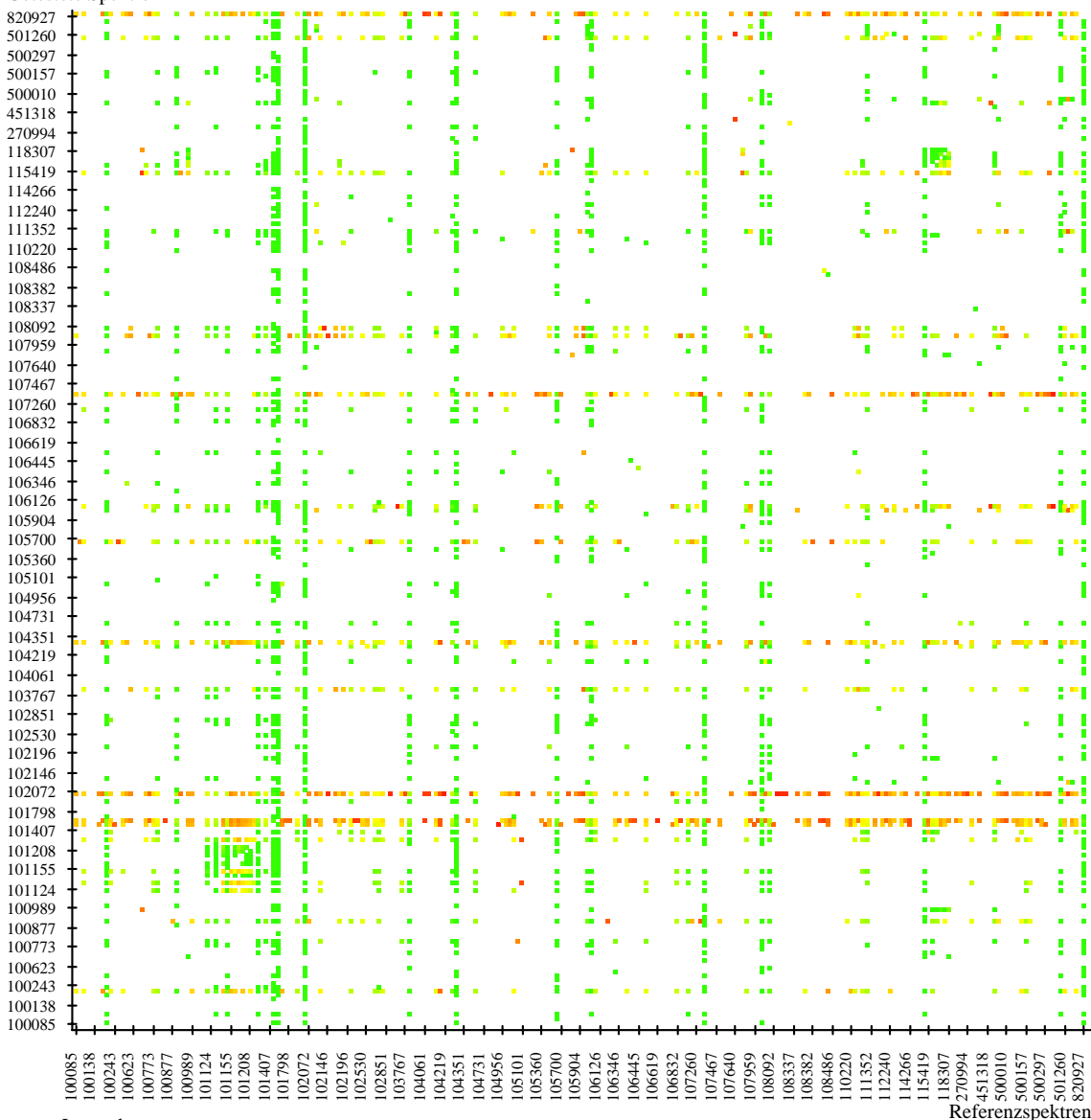
Algorithm: Standard
 No. of used factor sp.: -
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 3999.71
 To: 11999.1
 Order of Internal Derivation: 1
 Smoothing Points for Internal Derivation: 9



Ueberlapp. Ges.: 2988 (4.34 %) bei 196 (74.5 %) Spektren
 Ueberlapp. Max.: 143 bei 1 Spektren

wahr positiv: 65918 falsch negativ: 2988 Sensitivitaet: 95.664 %

Getestete Spektren



Legende:
 Relative Spektrale Distanz

0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

Abb. N28: Standardmethode (Vektornormierung und 1. Ableitung, Doppelkugelmodell, konstantes Konfidenzniveau von 99 %).