

7.4.5 Raman, Standardmethode

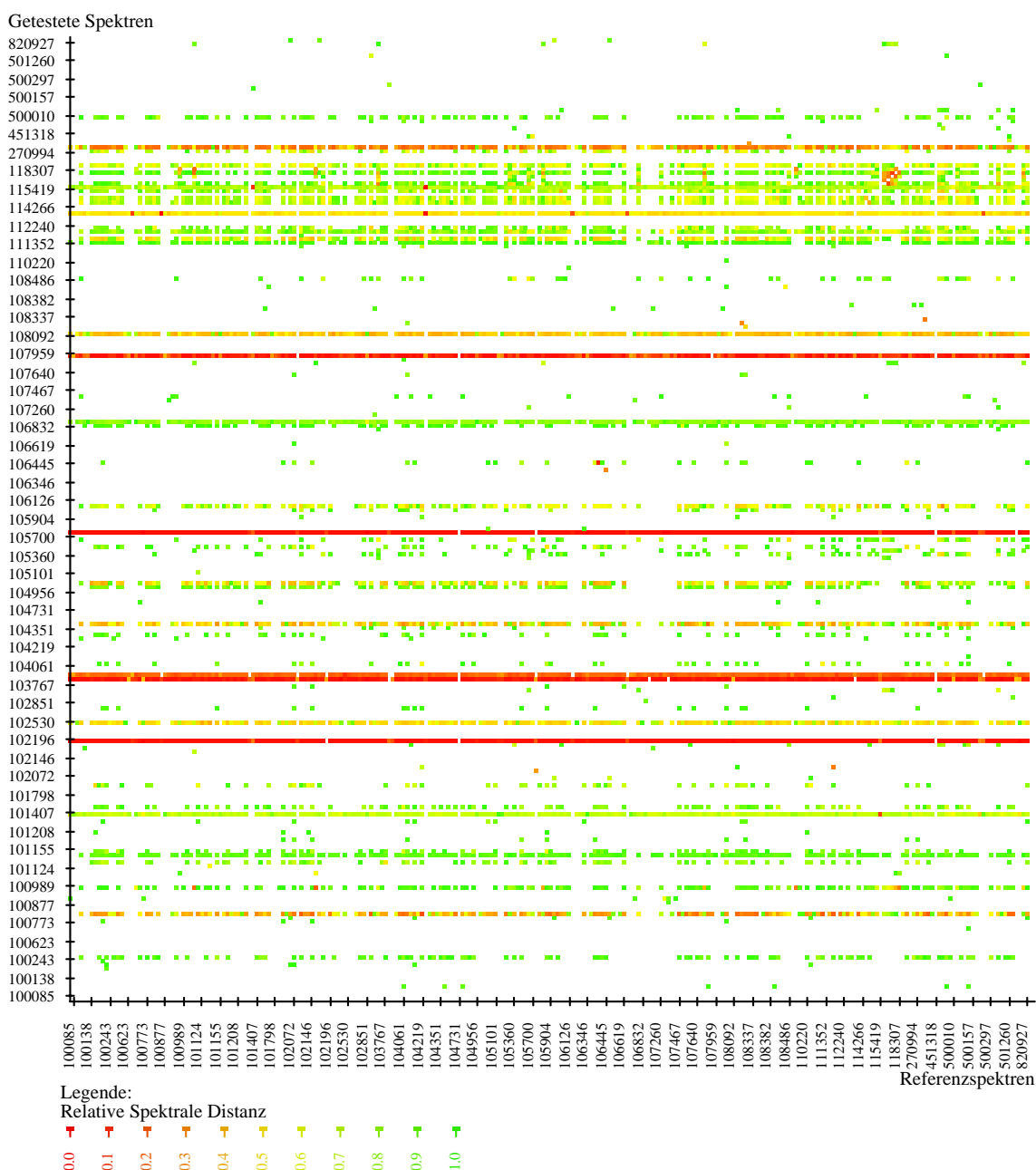
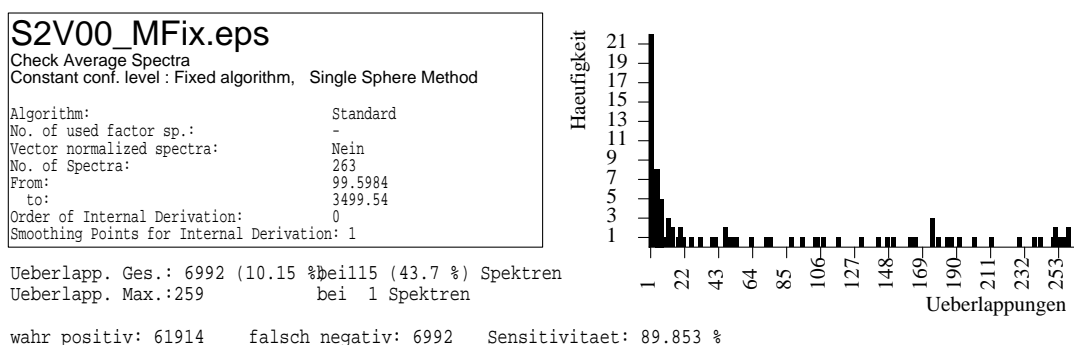
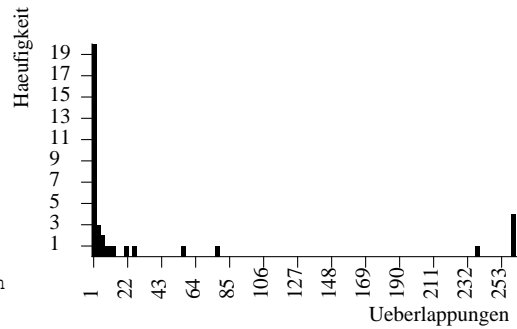


Abb. R1: Standardmethode.

```

snavl_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:                                     99.5984
to:                                       3499.54
Order of Internal Derivation:              0
Smoothing Points for Internal Derivation:  1
    
```



Ueberlapp. Ges.: 1555 (2.26 %) bei 44 (16.7 %) Spektren
 Ueberlapp. Max.: 260 bei 4 Spektren

wahr positiv: 67351 falsch negativ: 1555 Sensitivitaet: 97.743 %

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. R2: Standardmethode (Vektornormierung).

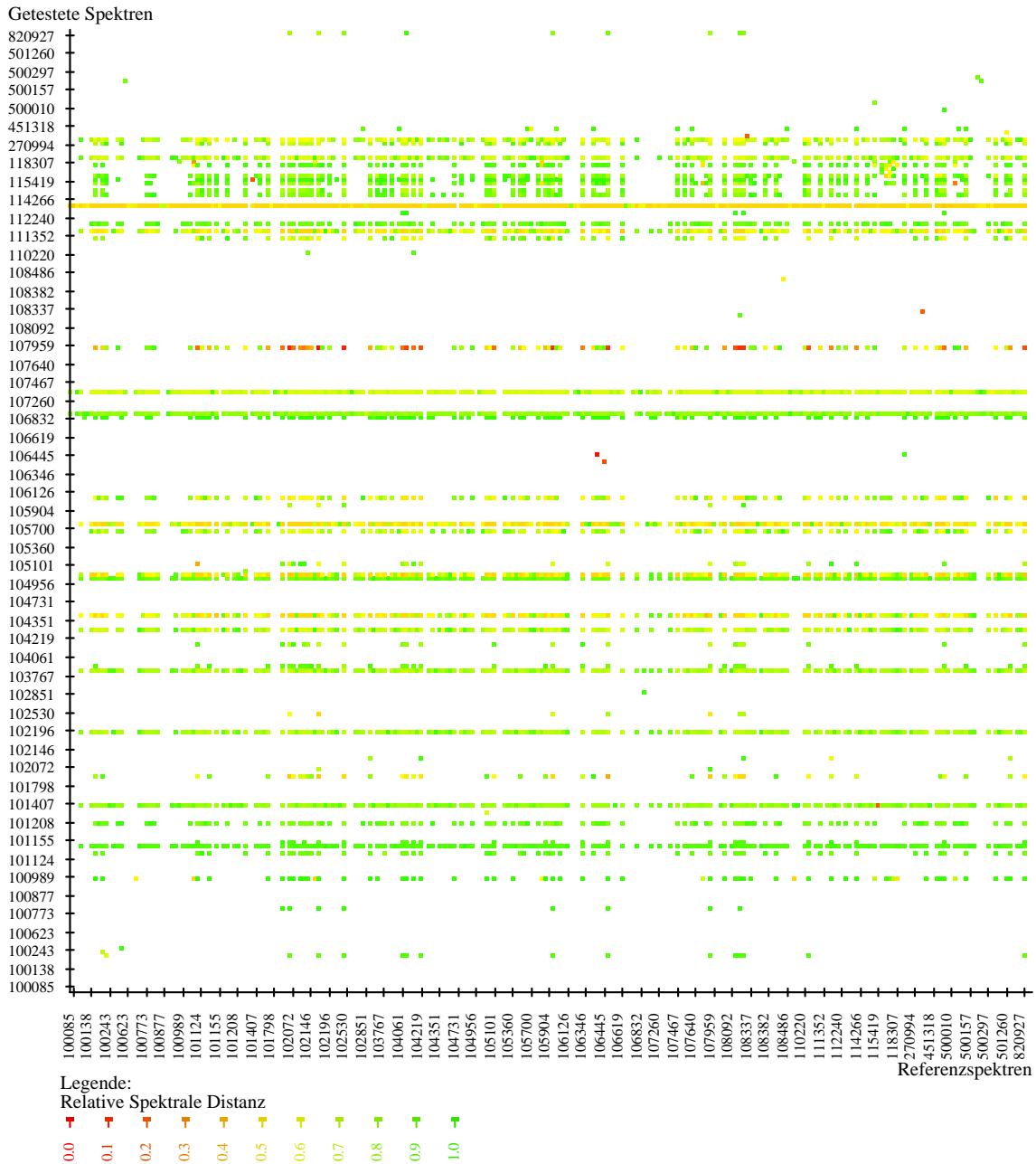
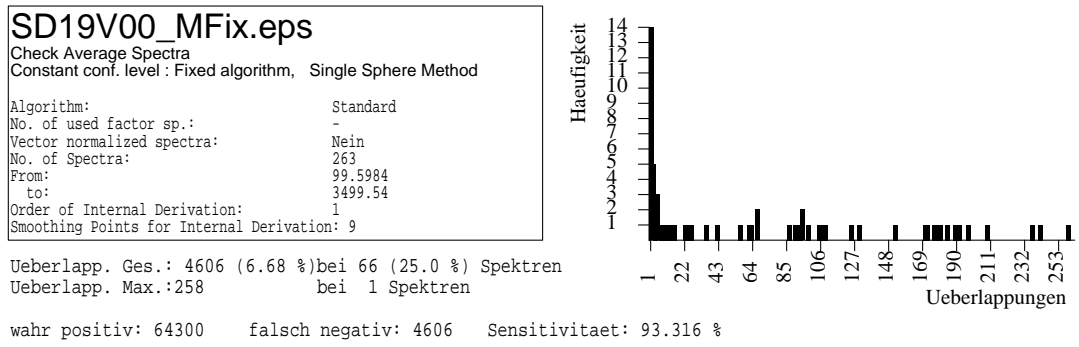


Abb. R3: Standardmethode (1. Ableitung).

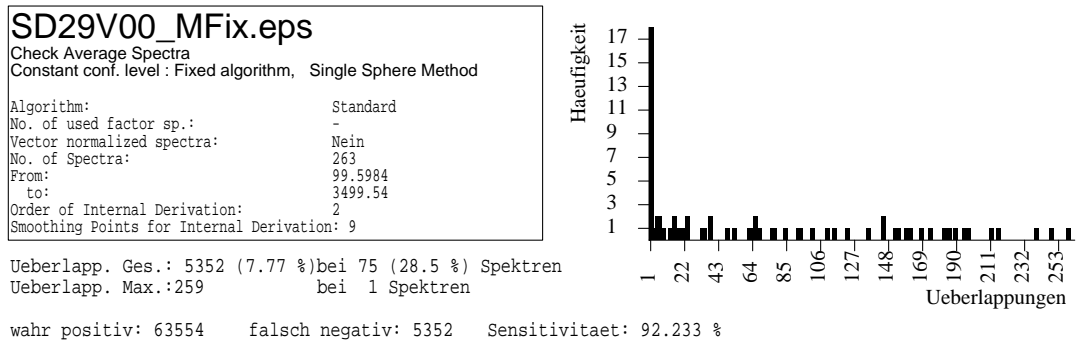
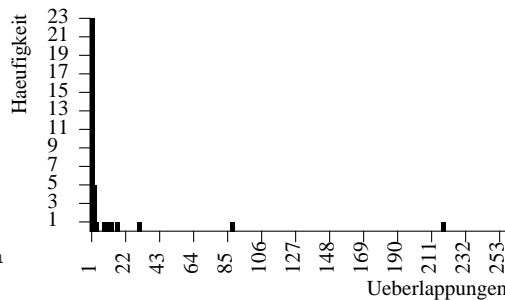


Abb. R4: Standardmethode (2. Ableitung).

SND19bVAL_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: 99.5984
 to: 3499.54
 Order of Internal Derivation: 1
 Smoothing Points for Internal Derivation: 9



Ueberlapp. Ges.: 1718 (2.49 %) bei 42 (15.9 %) Spektren
 Ueberlapp. Max.: 260 bei 5 Spektren

wahr positiv: 67188 falsch negativ: 1718 Sensitivitaet: 97.507 %

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. R5: Standardmethode (Vektornormierung und 1. Ableitung).

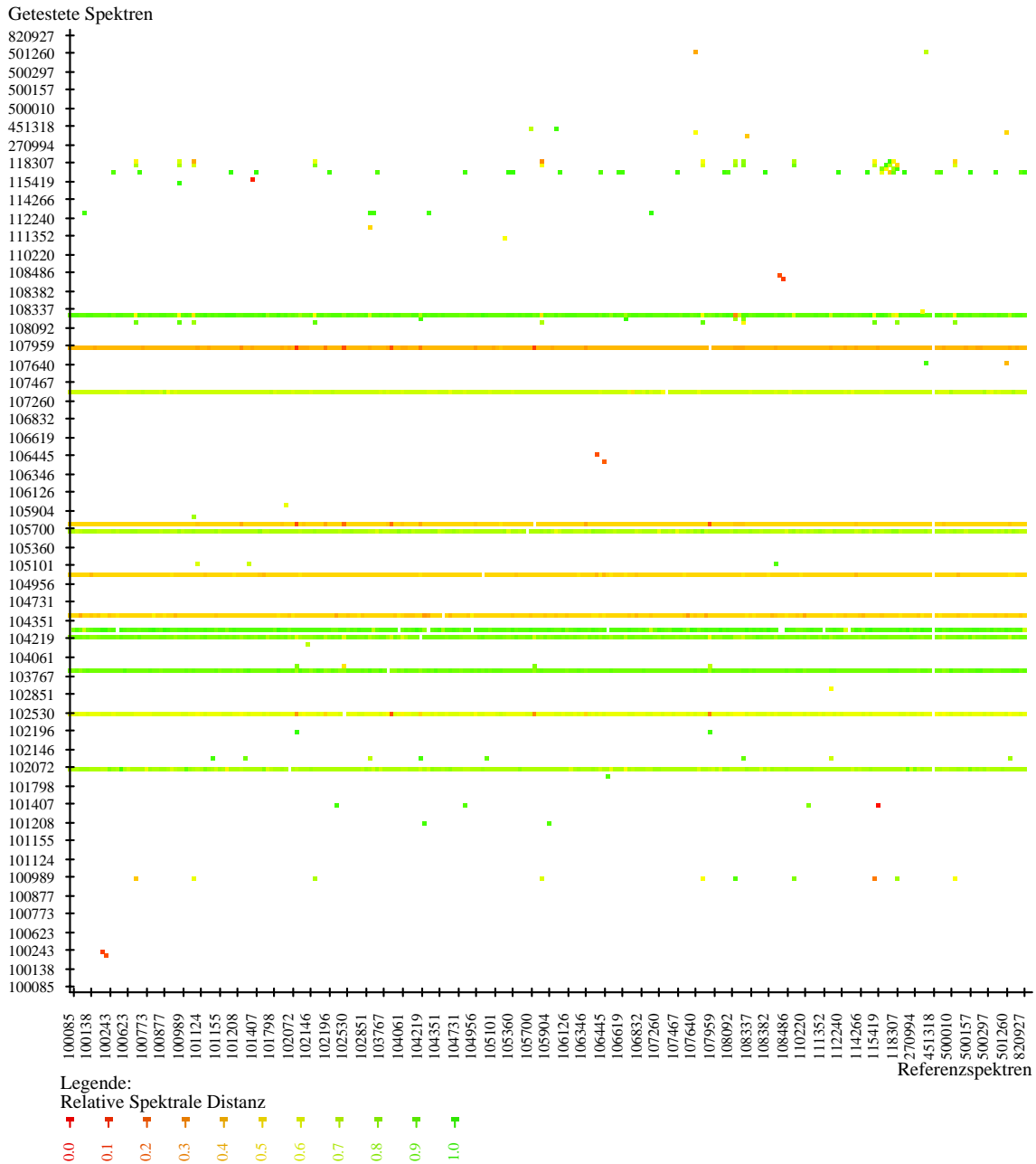
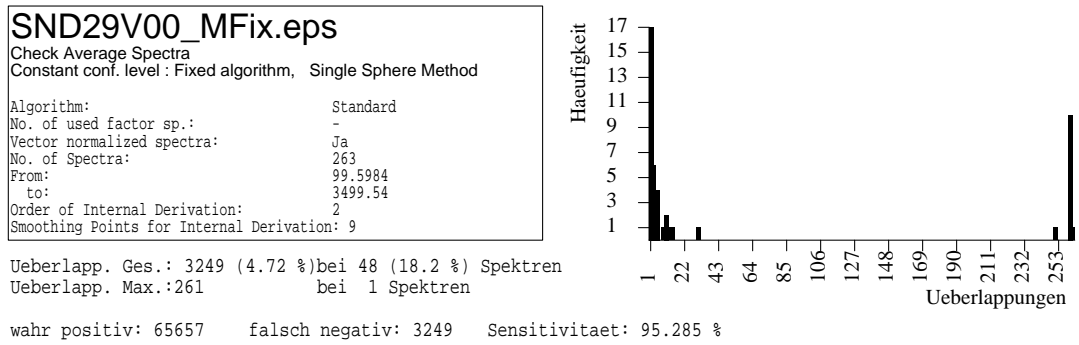
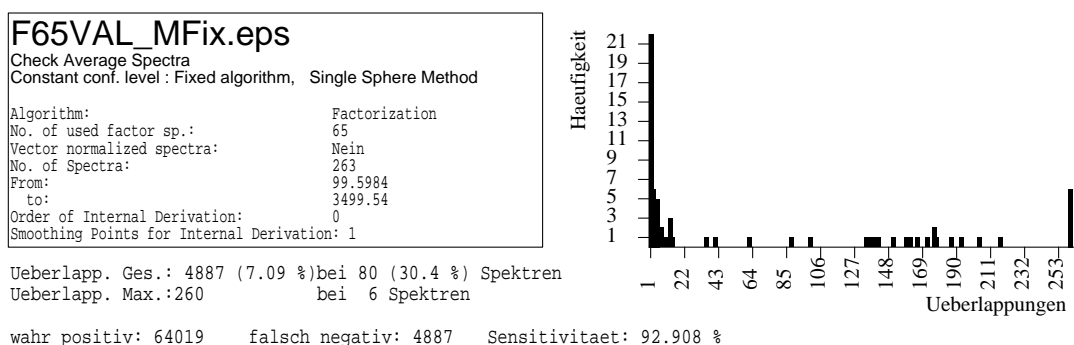


Abb. R6: Standardmethode (Vektornormierung und 2. Ableitung).

7.4.6 Raman, Faktormethode



Getestete Spektren

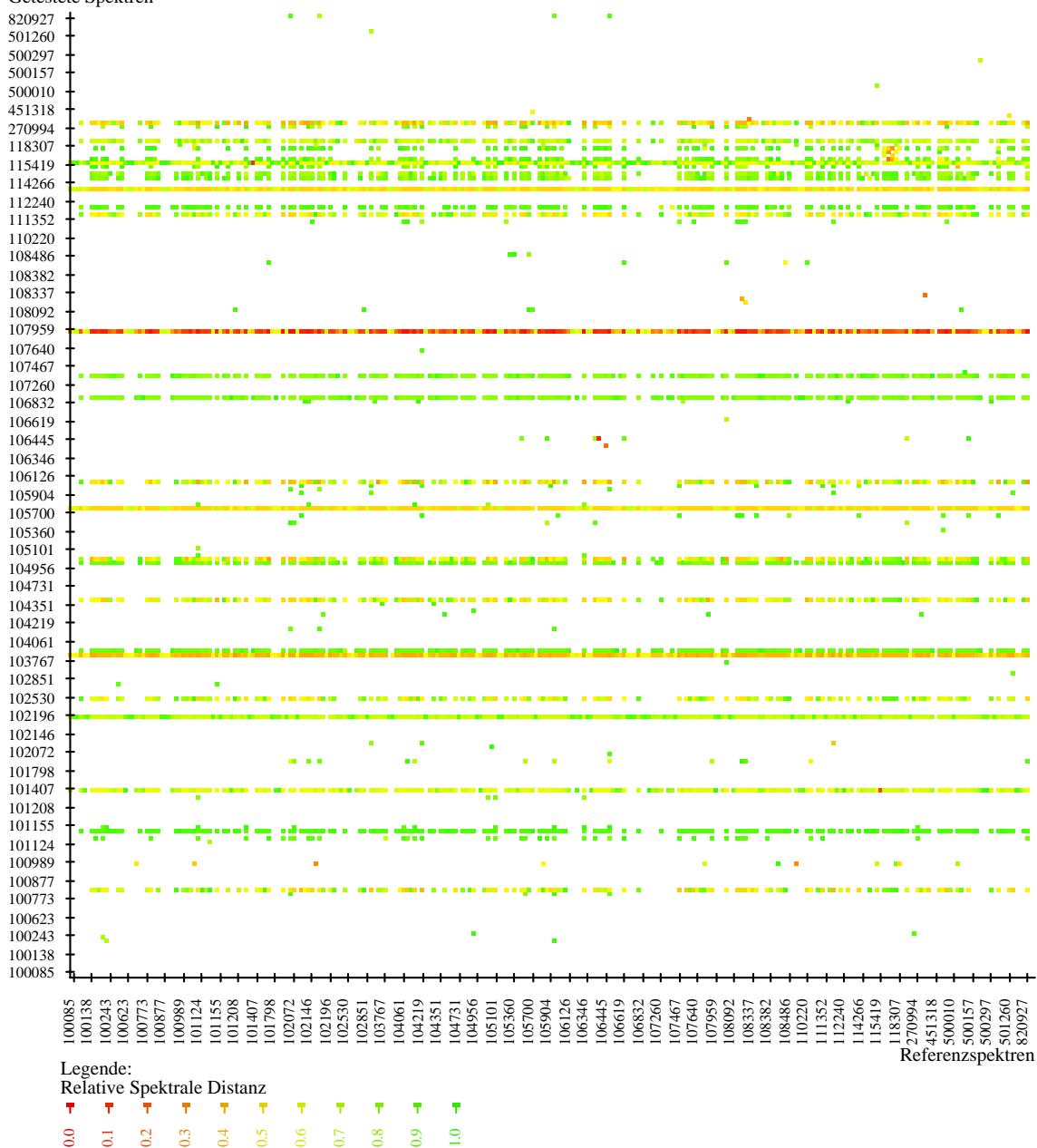
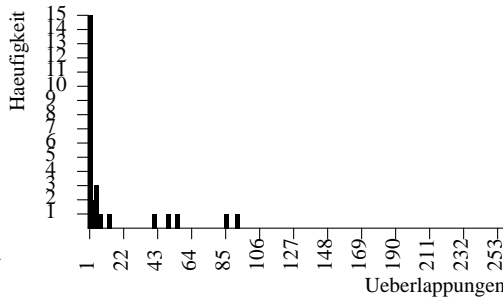


Abb. R7: Faktormethode (65 Faktoren).

F65NVAL_MFix.eps
 Check Average Spectra
 Constant conf. level: Fixed algorithm, Single Sphere Method

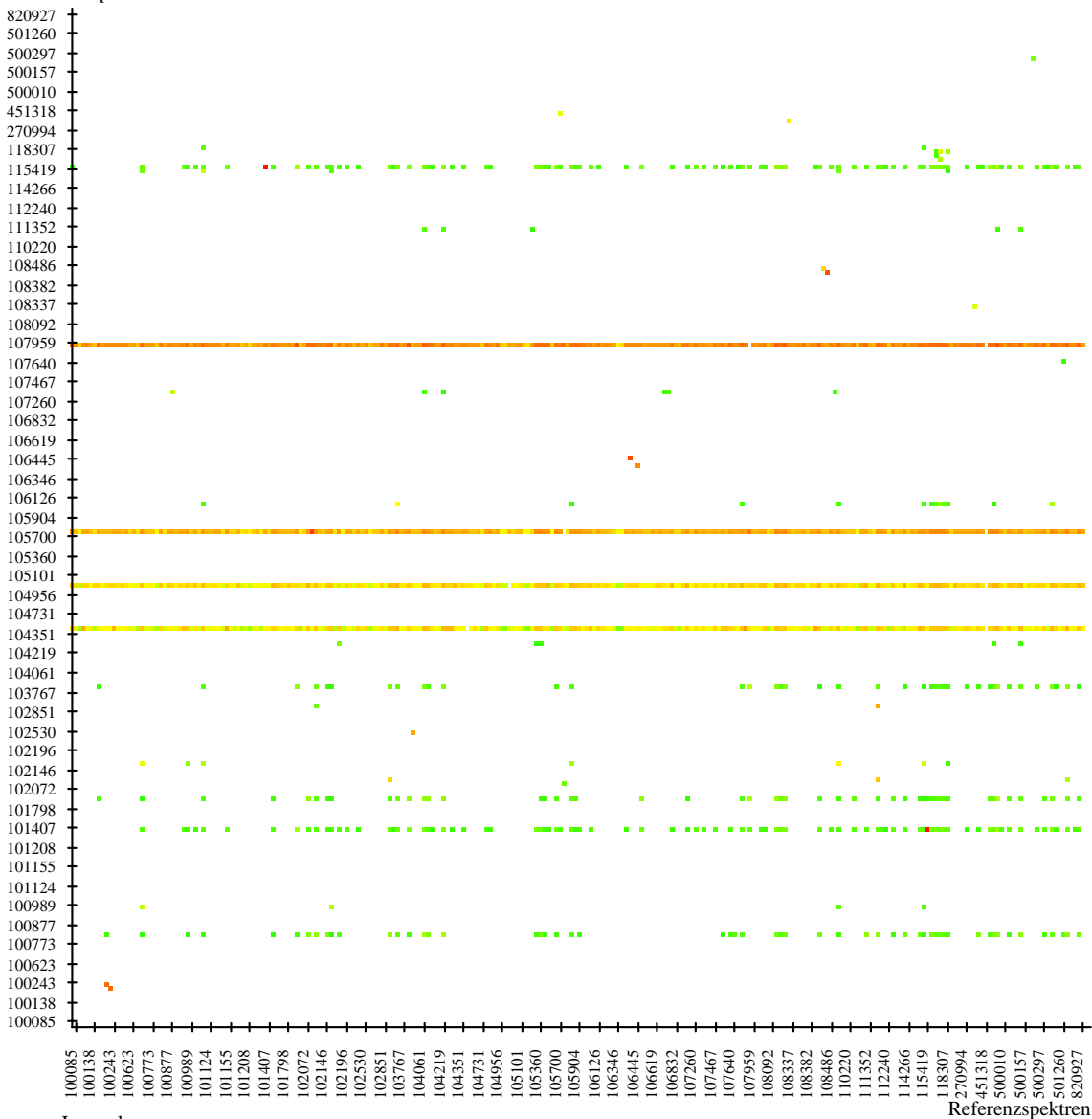
Algorithm: Factorization
 No. of used factor sp.: 65
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 99.5984
 to: 3499.54
 Order of Internal Derivation: 0
 Smoothing Points for Internal Derivation: 1



Ueberlapp. Ges.: 1430 (2.08 %) bei 36 (13.6 %) Spektren
 Ueberlapp. Max.: 260 bei 4 Spektren

wahr positiv: 67476 falsch negativ: 1430 Sensitivitaet: 97.925 %

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. R8: Faktormethode (65 Faktoren, Vektornormierung).

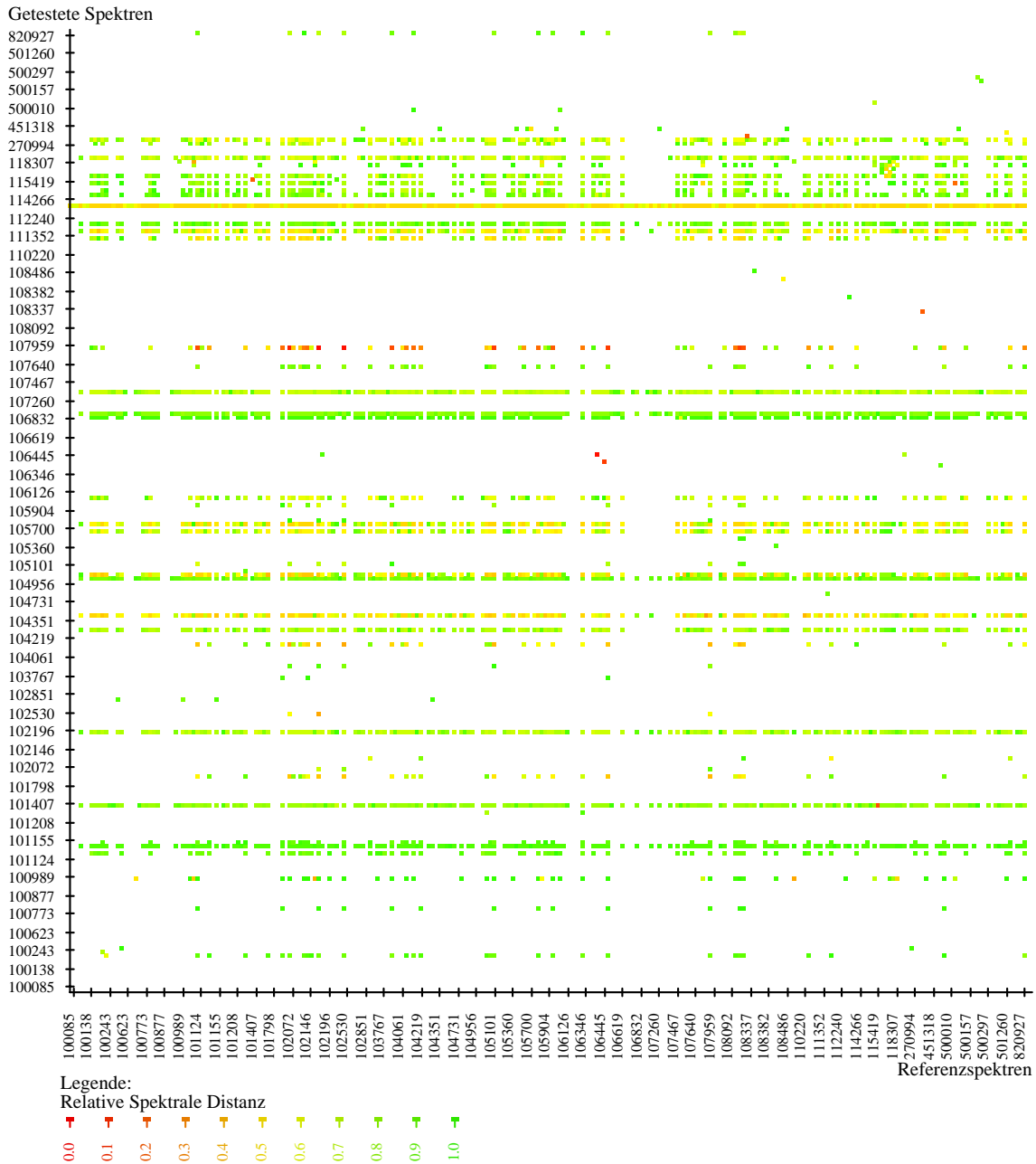
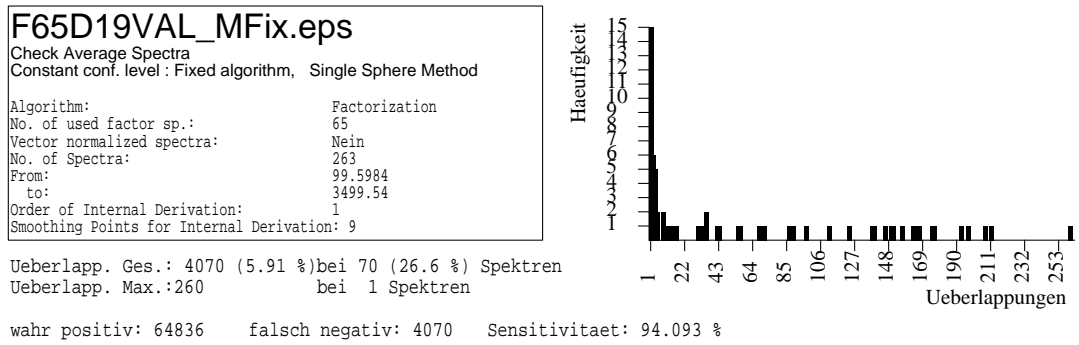
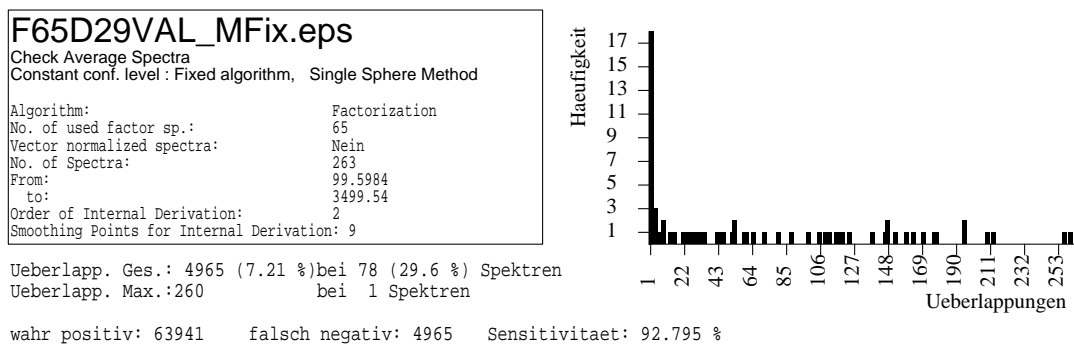


Abb. R9: Faktormethode (65 Faktoren, 1. Ableitung).



Getestete Spektren

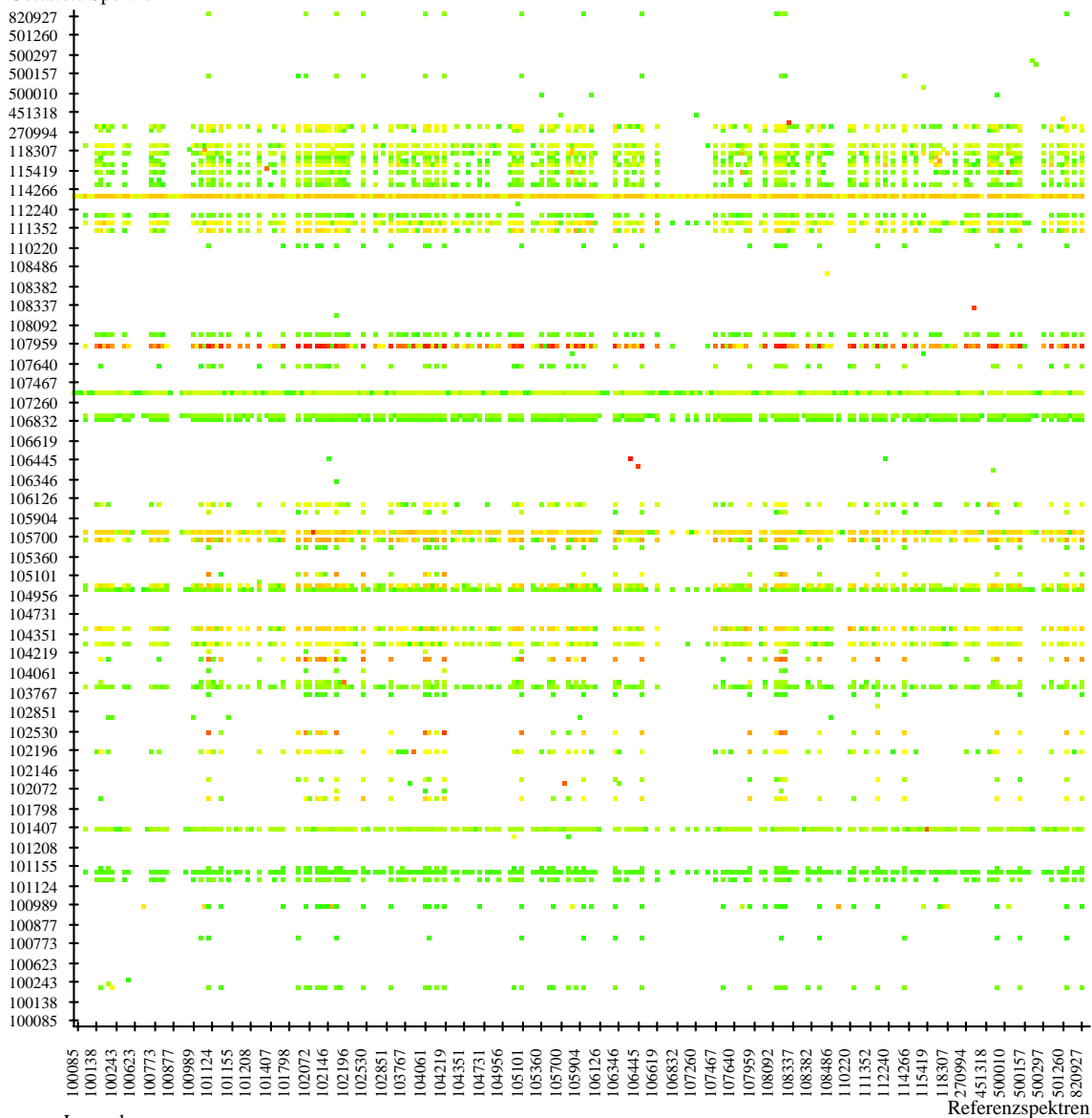
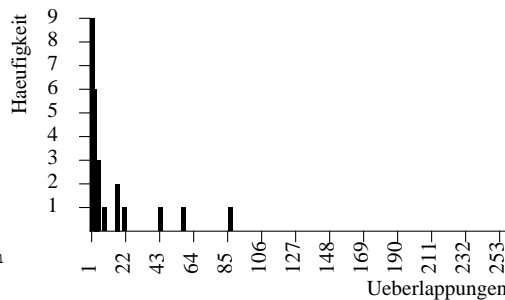


Abb. R10: Faktormethode (65 Faktoren, 2. Ableitung).

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

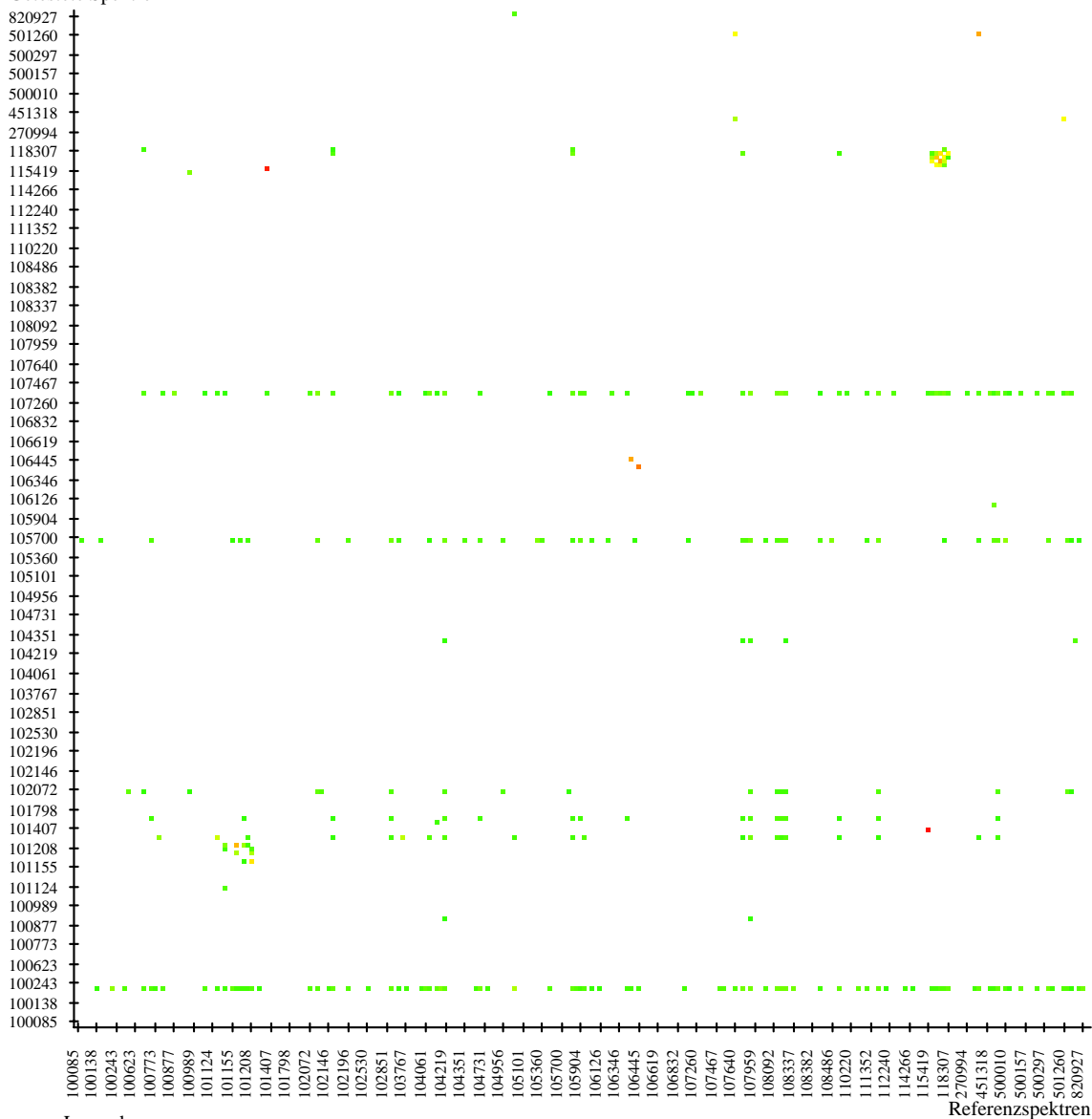
Algorithm: Factorization
 No. of used factor sp.: 65
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 3999.71
 to: 11999.1
 Order of Internal Derivation: 1
 Smoothing Points for Internal Derivation: 9



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. R11: Faktormethode (65 Faktoren, Vektornormierung, 1. Ableitung).

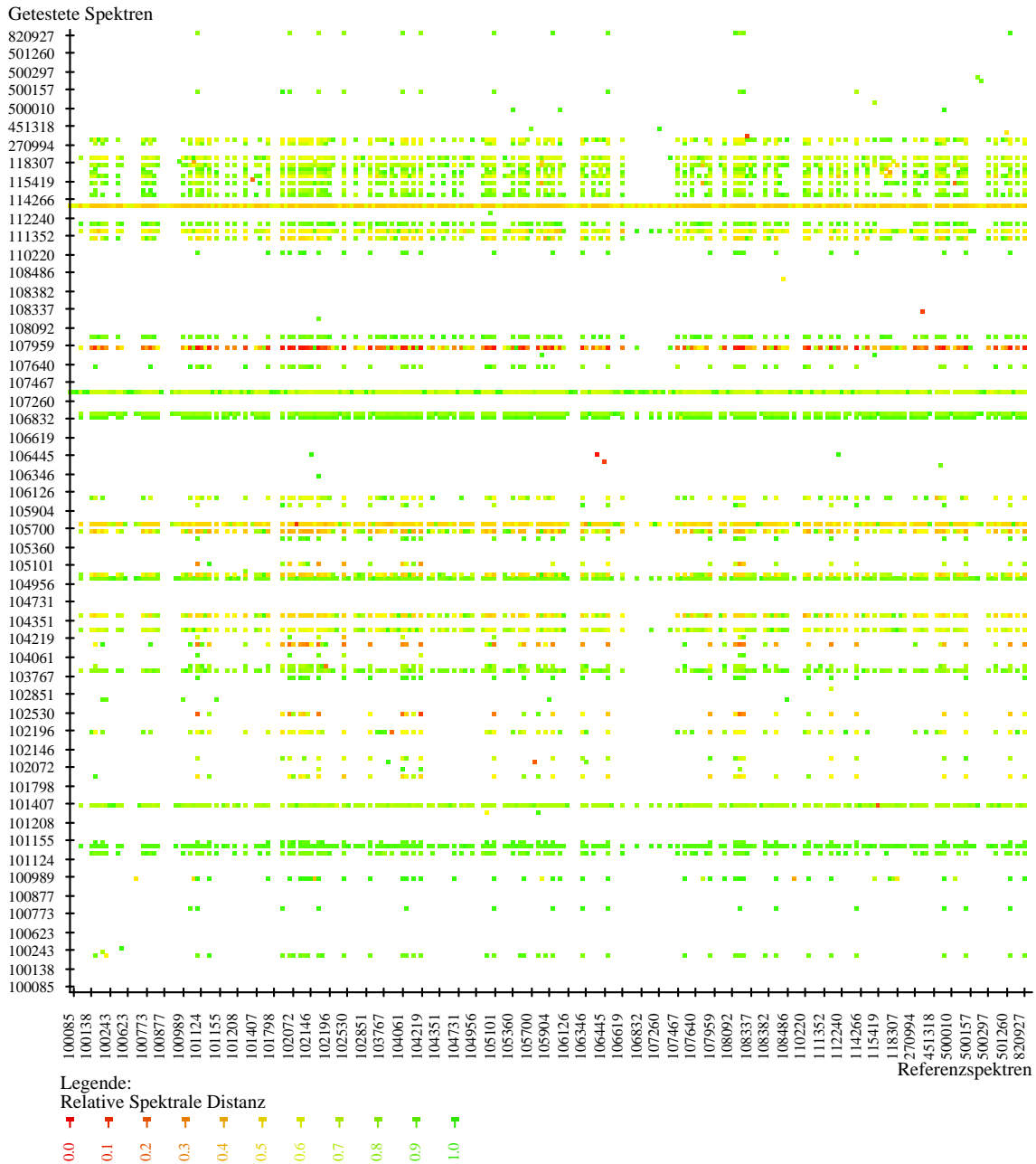
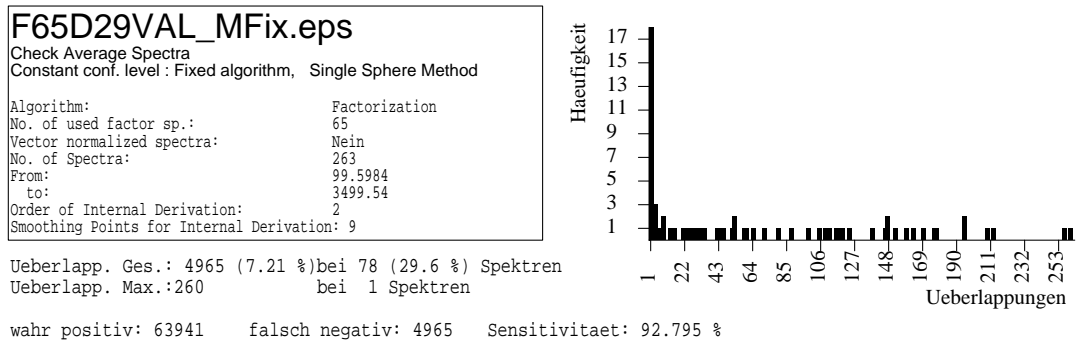
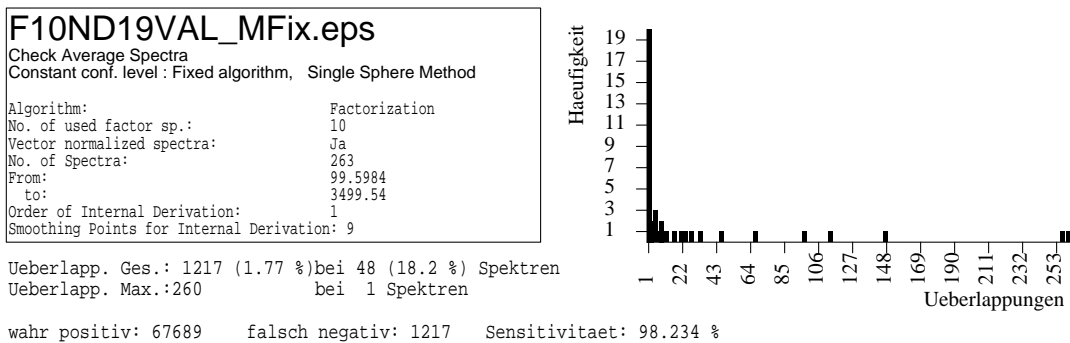


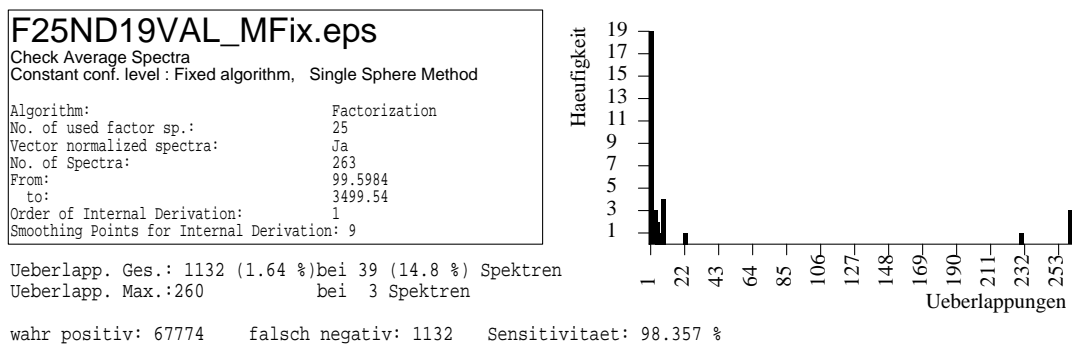
Abb. R12: Faktormethode (65 Faktoren, Vektornormierung, 2. Ableitung).



Getestete Spektren



Abb. R13: Faktormethode (10 Faktoren, Vektornormierung, 1. Ableitung).



Getestete Spektren



Abb. R14: Faktormethode (25 Faktoren, Vektornormierung, 1. Ableitung).

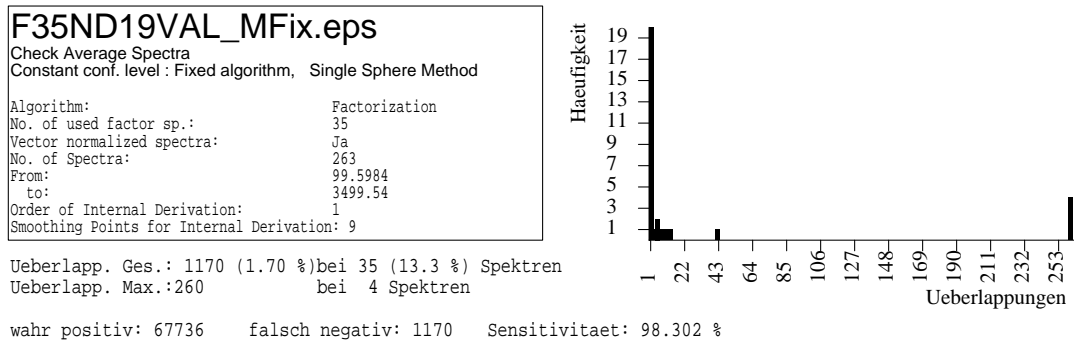
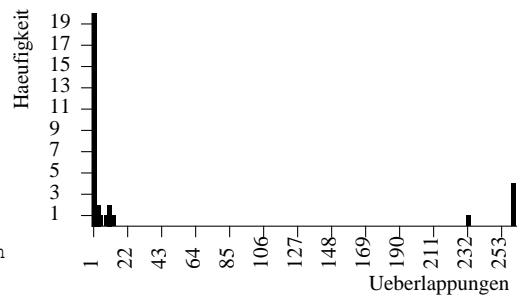


Abb. R15: Faktormethode (35 Faktoren, Vektornormierung, 1. Ableitung).

F45ND19VAL_MFix.eps
 Check Average Spectra
 Constant conf. level: Fixed algorithm, Single Sphere Method

Algorithm: Factorization
 No. of used factor sp.: 45
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 99.5984
 to: 3499.54
 Order of Internal Derivation: 1
 Smoothing Points for Internal Derivation: 9



Ueberlapp. Ges.: 1348 (1.96 %) bei 34 (12.9 %) Spektren
 Ueberlapp. Max.: 260 bei 4 Spektren

wahr positiv: 67558 falsch negativ: 1348 Sensitivitaet: 98.044 %

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. R16: Faktormethode (45 Faktoren, Vektornormierung, 1. Ableitung).

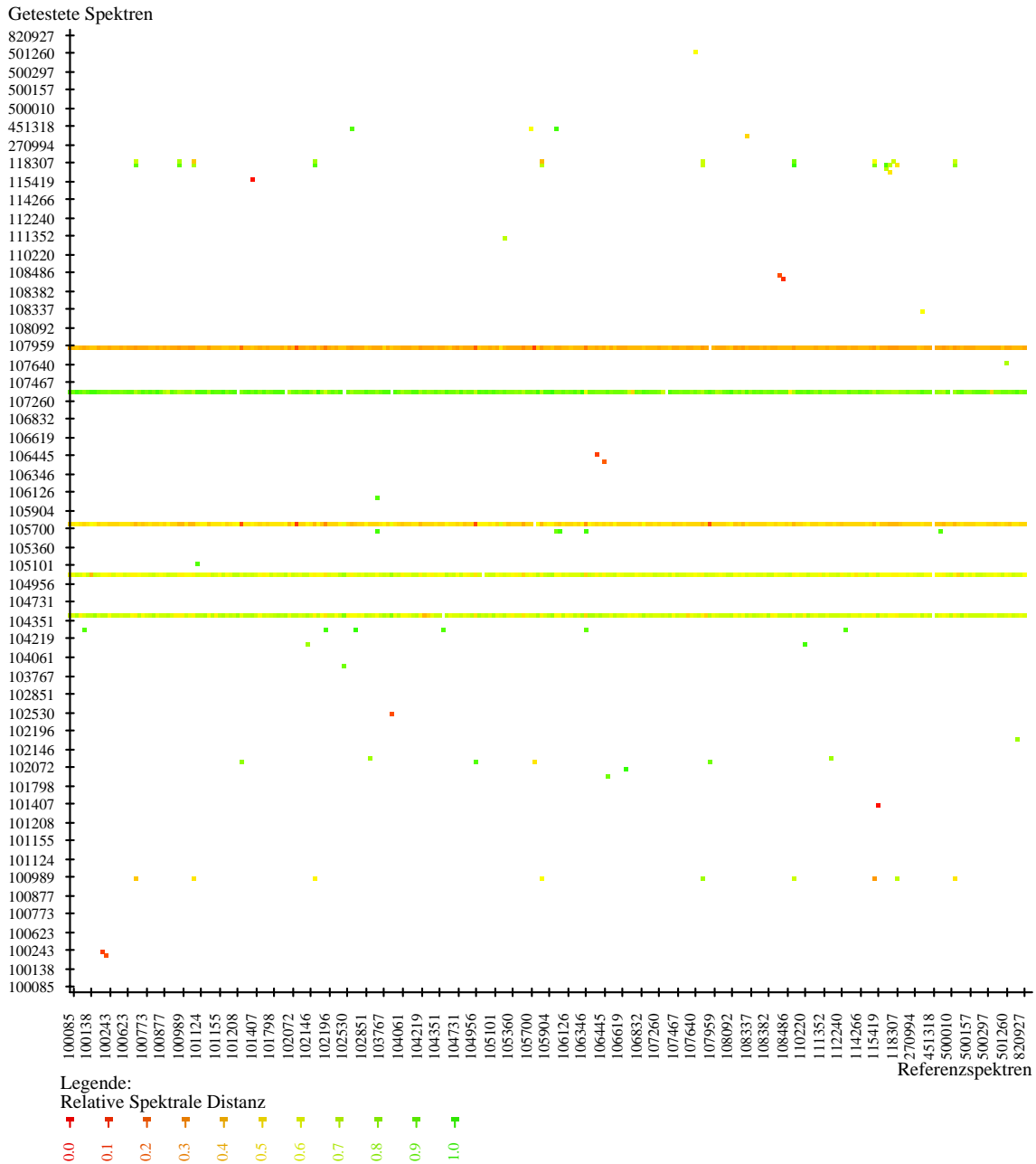
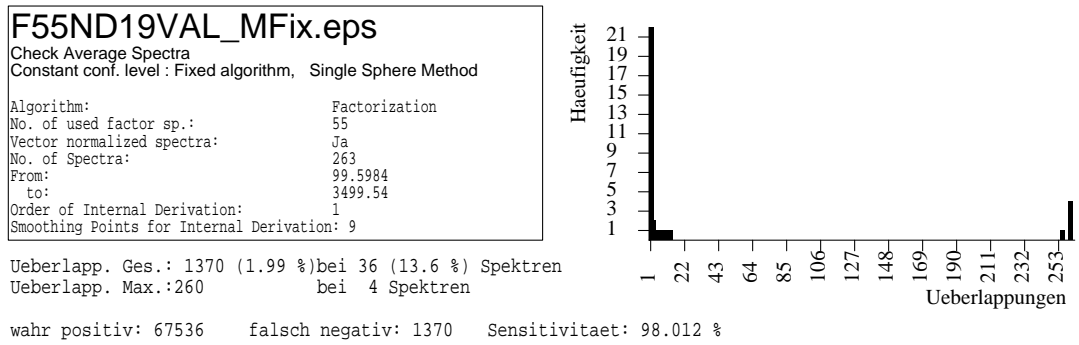
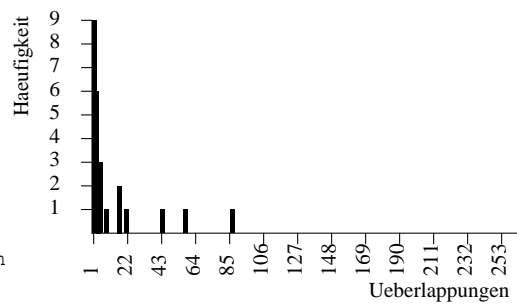


Abb. R17: Faktormethode (55 Faktoren, Vektornormierung, 1. Ableitung).

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

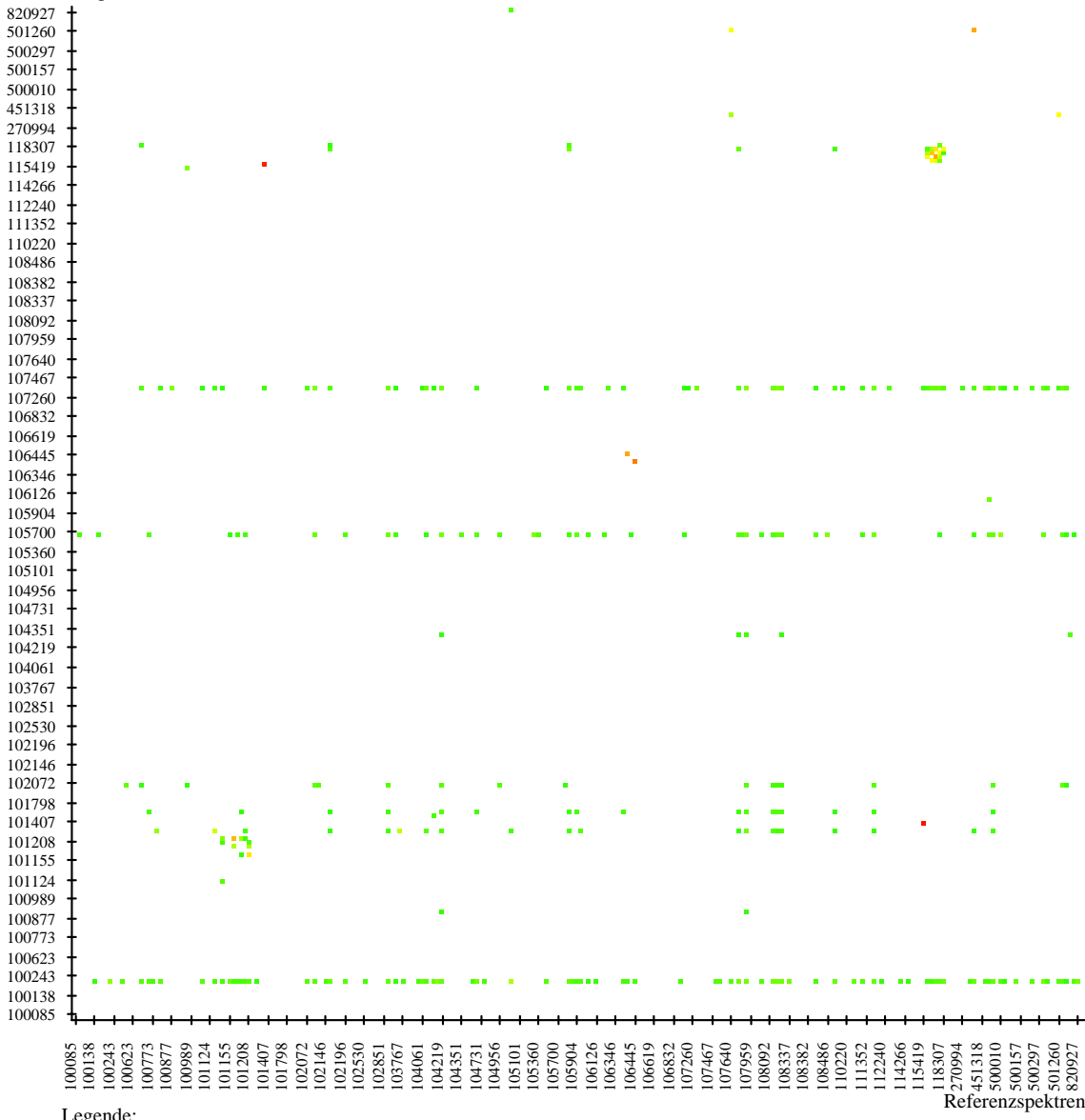
Algorithm: Factorization
 No. of used factor sp.: 65
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 3999.71
 To: 11999.1
 Order of Internal Derivation: 1
 Smoothing Points for Internal Derivation: 9



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. R18: Faktormethode (65 Faktoren, Vektornormierung, 1. Ableitung).

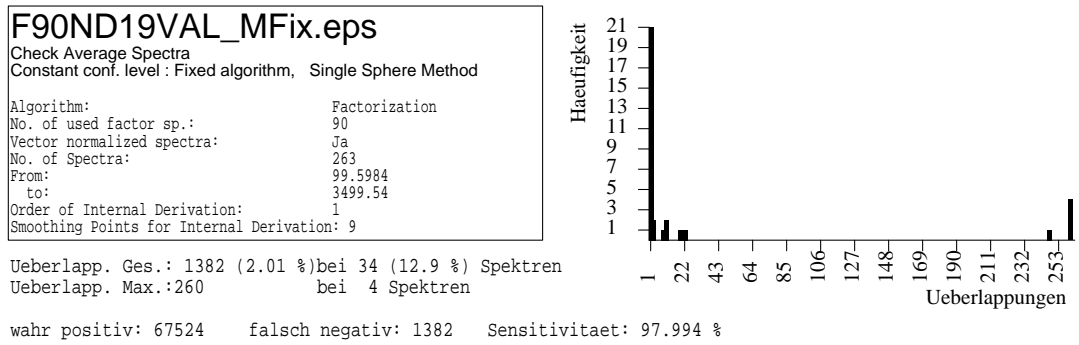
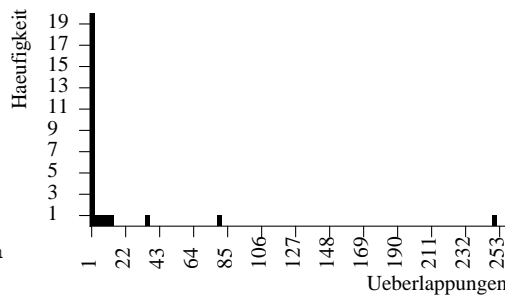


Abb. R19: Faktormethode (90 Faktoren, Vektornormierung, 1. Ableitung).

F120ND19VAL_MFix.eps
 Check Average Spectra
 Constant conf. level: Fixed algorithm, Single Sphere Method

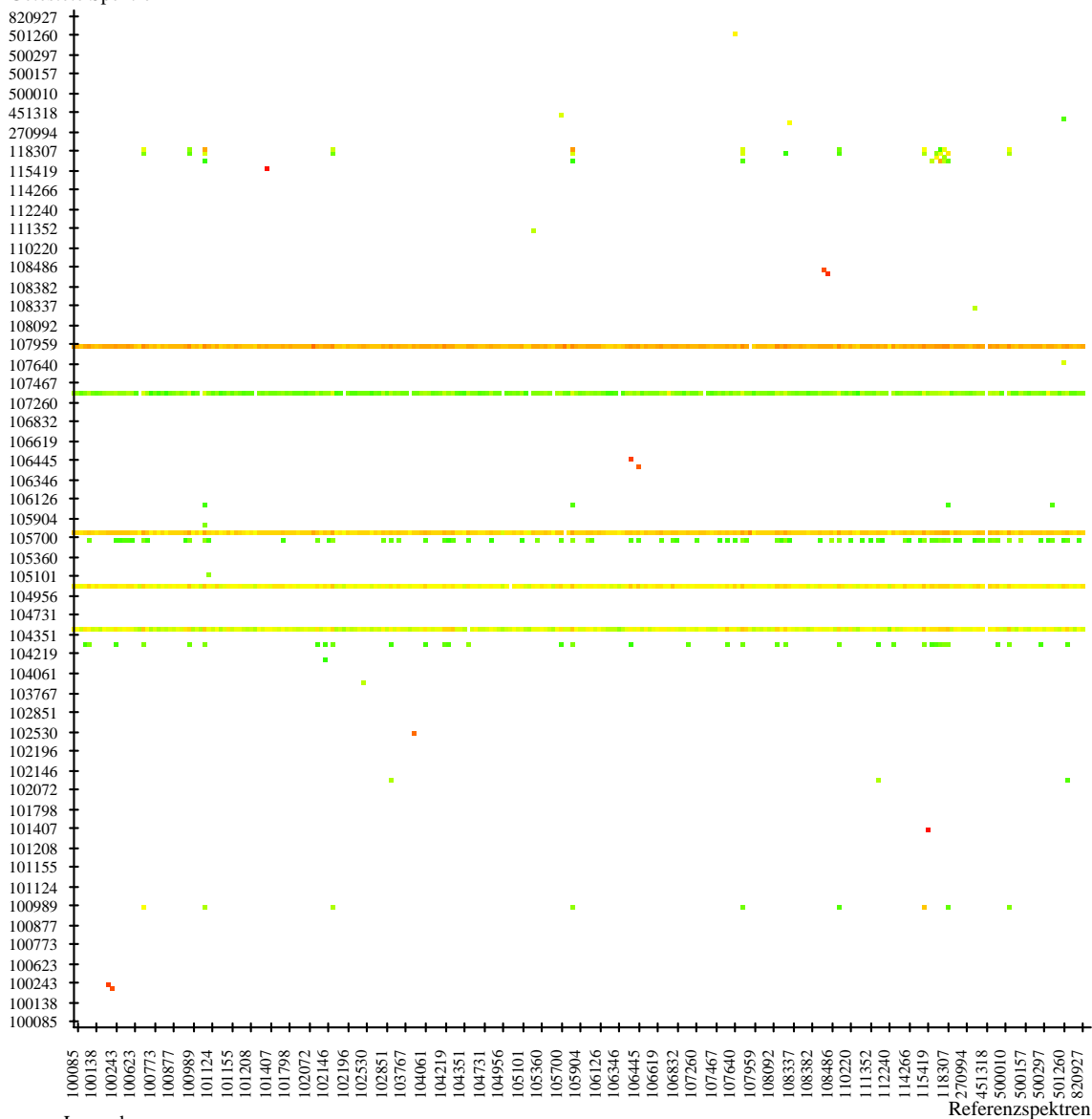
Algorithm: Factorization
 No. of used factor sp.: 120
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 99.5984
 to: 3499.54
 Order of Internal Derivation: 1
 Smoothing Points for Internal Derivation: 9



Ueberlapp. Ges.: 1472 (2.14 %) bei 35 (13.3 %) Spektren
 Ueberlapp. Max.: 260 bei 4 Spektren

wahr positiv: 67434 falsch negativ: 1472 Sensitivitaet: 97.864 %

Getestete Spektren

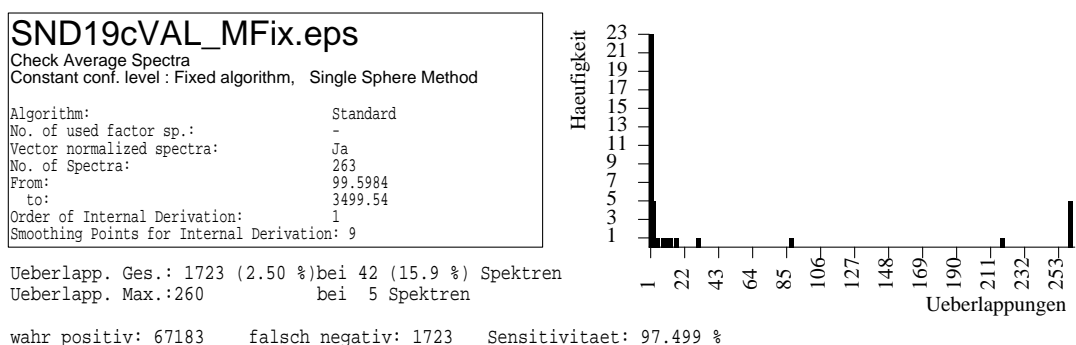


Legende:
 Relative Spektrale Distanz

0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

Abb. R20: Faktormethode (120 Faktoren, Vektornormierung, 1. Ableitung).

7.4.7 Raman, Variation des Spektralbereiches



Getestete Spektren

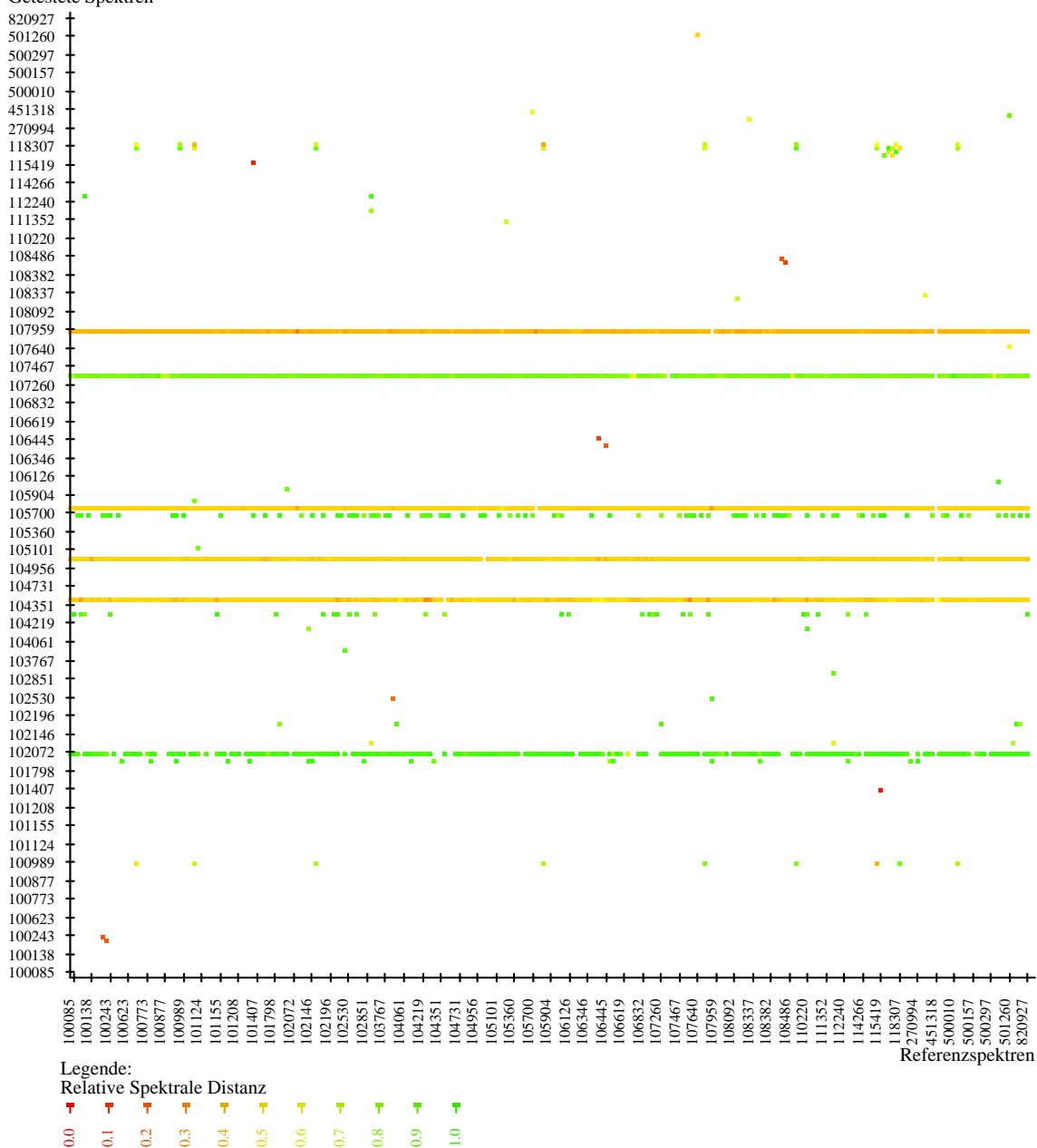
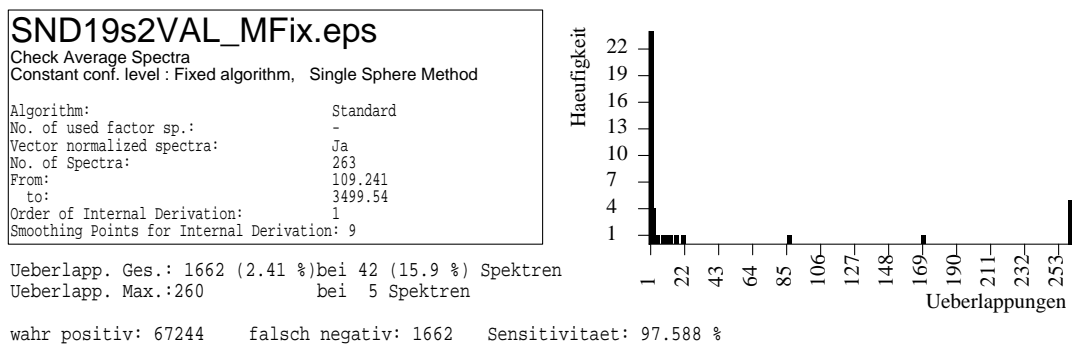


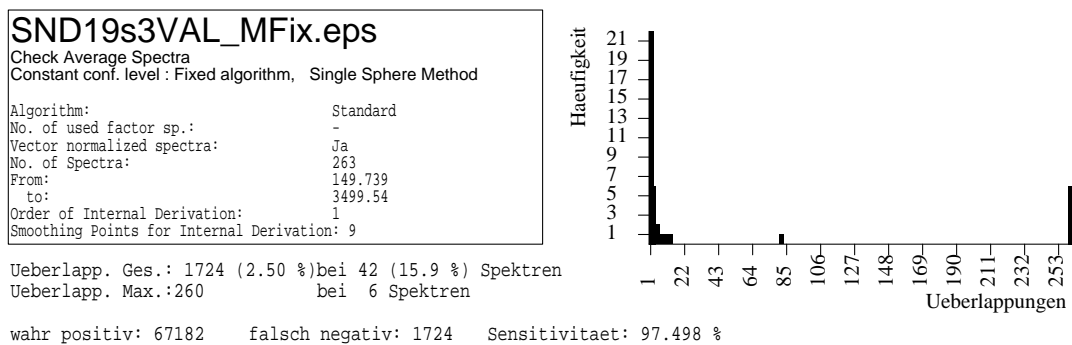
Abb. R21: Standardmethode (Vektornormierung, 1. Ableitung, 3500 cm^{-1} bis 100 cm^{-1}).



Getestete Spektren



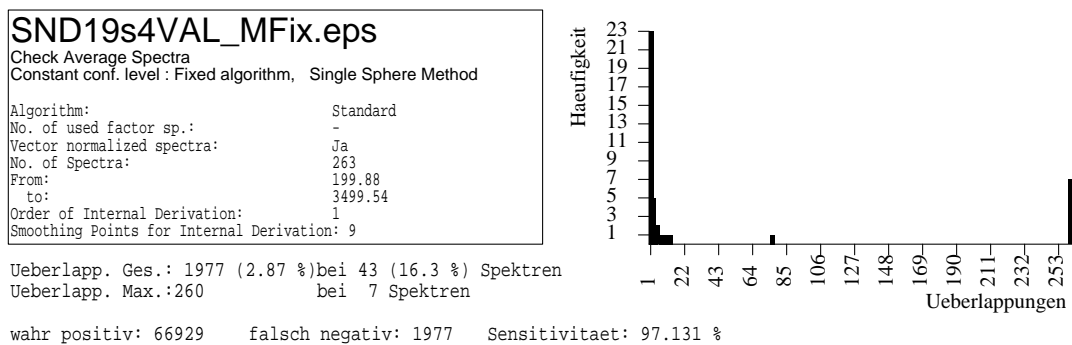
Abb. R22: Standardmethode (Vektornormierung, 1. Ableitung, 3500 cm^{-1} bis 110 cm^{-1}).



Getestete Spektren



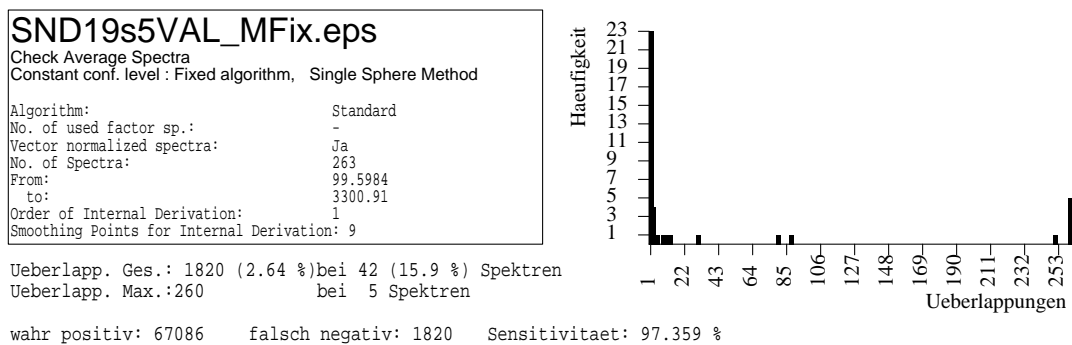
Abb. R23: Standardmethode (Vektornormierung, 1. Ableitung, 3500 cm^{-1} bis 150 cm^{-1}).



Getestete Spektren



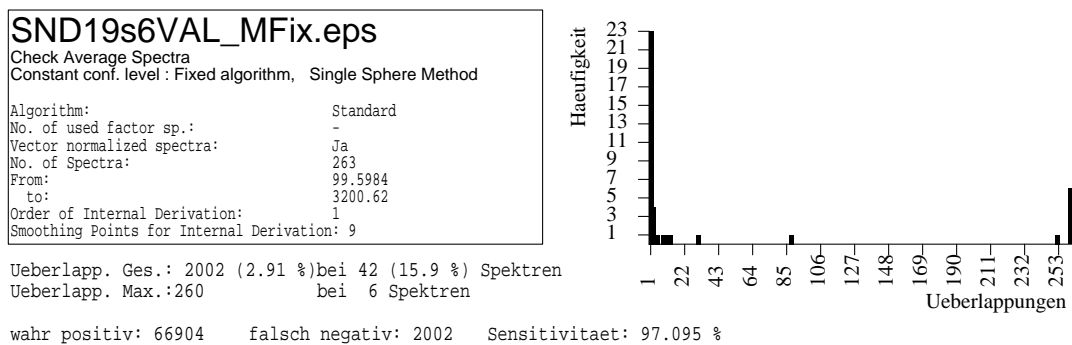
Abb. R24: Standardmethode (Vektornormierung, 1. Ableitung, 3500 cm^{-1} bis 200 cm^{-1}).



Getestete Spektren



Abb. R25: Standardmethode (Vektornormierung, 1. Ableitung, 3300 cm^{-1} bis 100 cm^{-1}).



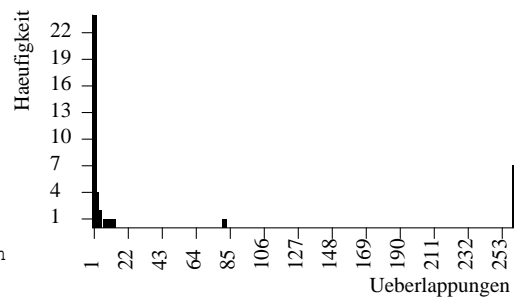
Getestete Spektren



Abb. R26: Standardmethode (Vektornormierung, 1. Ableitung, 3200 cm^{-1} bis 100 cm^{-1})

SND19s7VAL_MFix.eps
 Check Average Spectra
 Constant conf. level : Fixed algorithm, Single Sphere Method

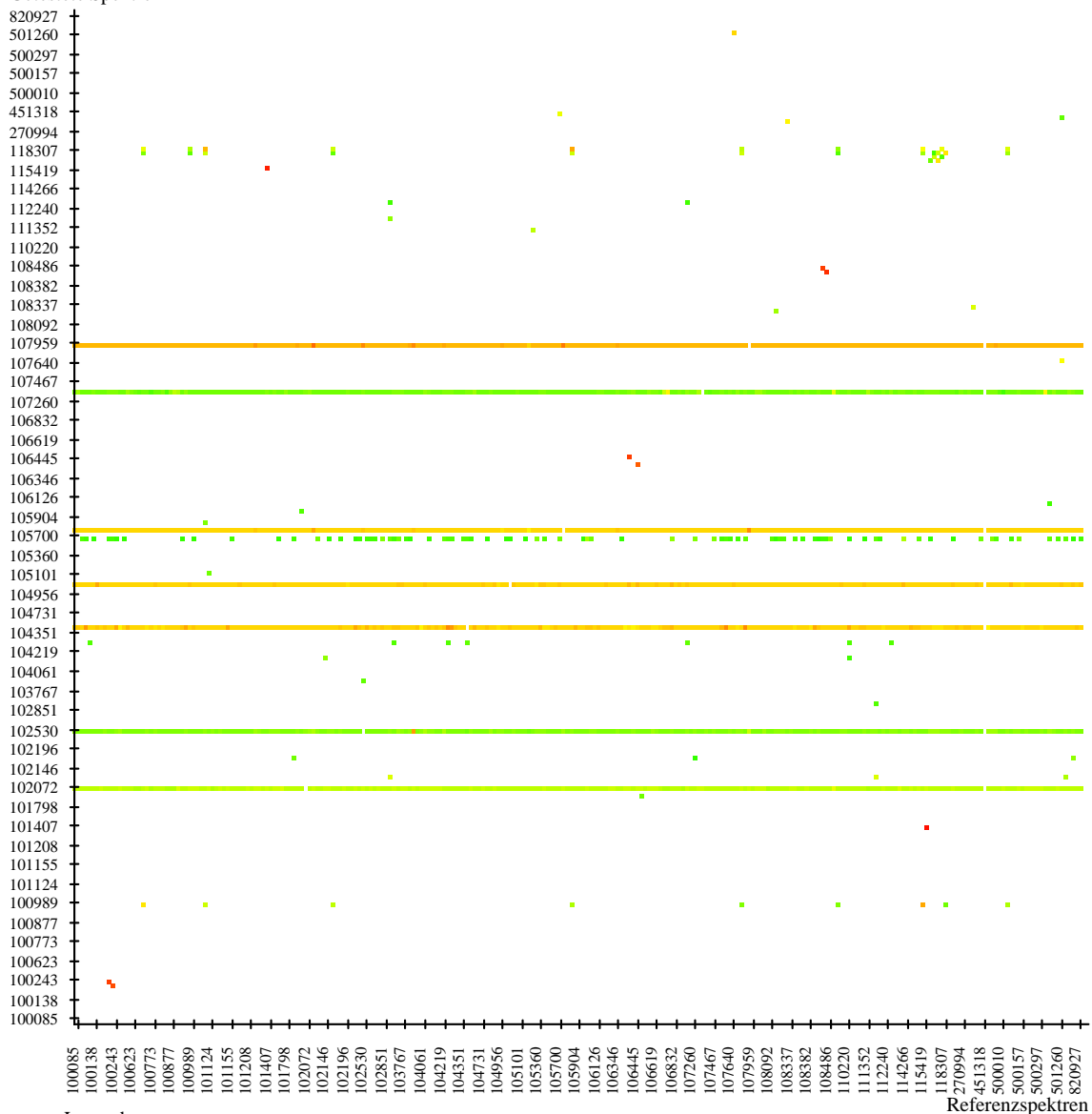
Algorithm: Standard
 No. of used factor sp.: -
 Vector normalized spectra: Ja
 No. of Spectra: 263
 From: 149.739
 to: 3200.62
 Order of Internal Derivation: 1
 Smoothing Points for Internal Derivation: 9



Ueberlapp. Ges.: 1977 (2.87 %) bei 42 (15.9 %) Spektren
 Ueberlapp. Max.: 260 bei 7 Spektren

wahr positiv: 66929 falsch negativ: 1977 Sensitivitaet: 97.131 %

Getestete Spektren



Legende:

Relative Spektrale Distanz



Abb. R27: Standardmethode (Vektornormierung, 1. Ableitung, 3200 cm^{-1} bis 150 cm^{-1})