7 Anhang

7.1 Software

Betriebssysteme:

- NT
- OS/2

Anwendungssoftware:

- OPUS-Ident (Bruker)
  Spektroskopie-Software mit „IDENT“-Erweiterung zur Erstellung von Spektrenbibliotheken
- Visual Studio 97 (Microsoft)
  Programmiersoftware, welche u.a. C++ umfaßt
- Matlab, Wavelet-toolbox (The Math Works Inc.)
  Software mit umfangreichen mathematischen Funktionen und Wavelet-Erweiterung zur Wavelet-Transformation mit Daubechies-Wavelets
- Specwork (C) 1997 von Dr. U. Depczynski,
  Software für die Wavelet-Transformation mit S-Wavelets

7.2 Substanzliste

Lfd.Nr. Art.Nr. Artikelname
1 100010 Acetanilid reinst krist
2 100085 Acetylsalicylsäure
3 100090 Adipinsäure reinst
4 100102 4-Aminobenzuesäure reinst
5 100103 Amidoschwefelsäure z.A.
6 100129 L-Asparaginsäure reinst
7 100130 Benzoesäure gepulvert
8 100138 3,5-Dinitrobenzoesäure
9 100162 Borsäure gepulvert reinst
10 100163 Di-Bortrioxid
11 100241 Citronensäure wasserfrei
12 100242 Citronensäure Monohydrat krist
13 100243 Citronensäure Monohydrat gepulvert
14 100289 L-Glutamin f. bioch. Zwecke
15 100290 L-Glutaminsäure reinst
16 100383 DL-Äpfelsäure, Lebensmittelqualität
17 100492 Oxalsäure-Dihydrat reinst
18 100623 Pikrinsäure z.A. (0,5ml Wasser/g)
19 100631 Salicylsäure reinst
20 100662 Sorbinsäure
21 100671 Stearinsäure
22 100668 Bernsteinsäure z.A.
23 100773 Tannin gepulvert rein
24 100802 L+Weinsäure krist
25 100807 Trichloressigsäure
26 100846 Adonit (Ribit) f.d. Mikrobiol.
27 100848 Aesculin rein
28 100877 Ethyl-4-aminobenzoat (Benzocain), reinst
29 100886 Ethyl-4-hydroxybenzoat Natriumsalz
30 100887 Ethyl-4-hydroxybenzoat
31 100944 Etylendinitrilotetra-Essigsäure reinst
32 100963 DL-Alanin für bioch. Zwecke
33 100989 Cetylalkohol (1-Hexadecanol) reinst
34 101005 1,1,1-Trichlor-2-Methyl-2-Propanol-Hemihydrat (Chlorbutanol)
35 101072 Aluminiumchloridhydroxid-Allantoin
36 101091 Aluminiumhydroxid gepulvert
37 101107 Aluminiumstearat
38 101124 Ammoniumdihydrogenphosphat reinst krist.
39 101125 Ammoniumbromid reinst
40 101131 Ammoniumhydrogencarbonat
41 101141 Ammoniumchlorid rein
42 101149 Ammoniumdichromat reist krist
43 101155 Di-Ammoniumhydrogencitrat reinst
44 101182 Ammoniumheptamolybdat-Tetrahydrat z.A.
45 101187 Ammoniumnitrat reinst
46 101190 Di-Ammoniumoxalat-Monohydrat
47101200 Ammoniumperoxodisulfat reinst
48 101208 Ammoniumthiosulfat LAB
49 101211 Ammoniumsulfat f. b. Zw.
50 101212 Ammoniumthiocyanat reinst
51 101218 di-Ammoniumhydrogenphosphat m. Fließmittel
52 101226 Ammoniummonovanadat z.A.
53 101407 Kristallviolett C.I. 42555
54 101492 L(+)-Araboise f. Mikrobiologie
55 101543 L-Argininmonohydrochlorid
56 101565 L-Asparagin-Monohydrat reinst
57 101719 Bariumchlorid-Dihydrat z.A.
58 101798 1H-Benzotriazol techn.
59 101838 Curco BS
60 101841 Oxalsäure-bis-(Cyclohexylidenhydrazid) z.A.
61 102070 Calciumchlorid 90-95% entwässert
62 102071 Calciumcarbonat f. op. Glas
63 102072 Calciumchlorid-Hexahydrat reinst
64 102102 Calciumlactat, löslich reinst
65 102110 Calciumhydroxid FCC Lebensmittelqualität
66 102127 Beta-Cyclodextrin
67 102144 Calciumhydrogenphosphat wasserfrei
68 102146 Calciumhydrogenphosphat Dihydrat
69 102148 Calcium-D-Saccharat reinst
70 102154 Calciumstearat
71 102162 Calciumsulfat Hemihydrat gebrannt
72 102166 D(-)-Campher raffiniert, gepulvert
73 102196 Hydroxylapatit f. Biokeramik
74 102352 Cellobiose f. bioch. Zwecke
75 102424 Chloramin T Trihydrat reinst
76 102425 Chloralhydrat
77 102507 Cinchoninhydrochlorid Monohydrat
78 102530 Cobalt-II-acetat Tetrahydrat
79 102584 Coffein rein
80 102836 L-Cystin reinst
81 102838 L-Cystein für bioch. Zwecke
82 102839 L-Cysteinhydrochlorid-Monohydrat für bioch. Zwecke
83 102851 Calciumlaevulinat reinst
84 102968 Neocuproin (2,9-Dimethyl-1,10-Phenanthrolin) z.A.
85 103006 Dextrin weiß
86 103149 (+-)-Ephedrinhydrochlorid
87 103672 Colesterin gepulvert
88 103767 Ammoniumformiat reinst
89 103883 Eisen-III-nitrat Nonahydrat z.A.
90 103929 Fluorescin-Natrium reinst
91 103962 Eisen(II)-fumarat, reinst
92 104005 Paraformaldehyd reinst

93 104061 D(+)-Galactose reinst
94 104078 Gelatine gepulvert
95 104112 Calciumglycerophosphathydrat
96 104128 Auxillin (Gibberillin mit etwa 90% wirks. Gibberillin A3)
97 104168 Beta-Glycerophosphat Dinatrium-salz-Pentahydrat
98 104219 Guanidiniumchlorid f. b. Zw.
99 104228 Gummi Arabisch, sprühgetrocknet
100 104343 Methenamin
101 104349 Homatropinmethylbromid
102 104350 L-Histidinmonohydrochlorid-Monohydrat f. b. Zw.
103 104351 L-Histidin f. b. Zw.
104 104370 Histamindihydrochlorid reinst
105 104506 L-Hydroxyprolin f. b. Zw.
106 104541 Dragiersuspension f. farbint. Dragees
107 104610 Hydrochinon Fotopur
108 104731 Myo-Inosit
109 104751 Jodoform gepulvert reinst
110 104819 Kalium-Titriplex Dihydrat z.A.
111 104820 Kaliumacetat reinst
112 104892 Kaliumhydrogentartrat reinst
113 104956 Tri-Kaliumcitrat-Monohydrat reinst
114 104982 Kaliumhexacyanoferrat-II-Trihydrat reinst
115 105061 Kaliumnitrat reinst
116 105072 Di-Kaliumoxalat-Monohydrat reinst
117 105099 Di-Kaliumhydrogenphosphat-Trihydrat z.AAv10
118 105101 Di-Kaliumhydrogenphosphat wasserfrei reinst
119 105102 Tri-Kaliumphosphat-Trihydrat reinst
120 105118 Kaliumsorbat Pulver
121 105125 Kaliumthiocyanat z.A.
122 105321 D-(-)-Fructose reinst
123 105360 L-Leucin
124 105362 L-Isoleucin
125 105645 DL-alpha-Liponsäure, reinst
126 105683 Trilithiumcitrat-Tetrahydrat
127 105691 Lithiumhydroxid
128 105700 L-Lysinmonohydrochlorid f. b. Zw.
129 105707 L-Methionin
130 105870 Magnesiumhydroxid, reinst
131 105873 Magnesiumperchlorat-Hydrat (ca. 83%-ig)
132 105876 Magnesiumstearat gefällt fein gepulvert
133 105904 Magnesiumcitrat, reinst
134 105911 Maltose Monohydrat, krist
135 105924 Mangan-II-carbonat-Hydrat z. A.
136 105984 D(+)-Mannose
137 105995 (-)-Menthol krist
138 106126 2-Morpholinoethansulfonsäure-Monohydrat
139 106129 3-Morpholinopropansulfonsäure
140 106223 1-Naphthol
141 106247 Naphazolinnitrat, reinst
142 106249 Naphazolinhydrochlorid, reinst
143 106346 Natriumdihydrogenphosphat-Monohydrat z.A.
144 106371 Natriumborhydrid z.A.
145 106392 Natriumcarbonat wasserfrei
146 106431 Tri-Natriumcitrat-5,5-Hadrat reinst
147 106432 Tri-Natriumcitrat-Dihydrat
148 106445 Natrium-L-glutamat-Monohydrat
149 106446 tri-Natriumcitrat Dihydrat gepulvert reinst
150 106467 Natriumhydroxid granuliert
151 106544 Natriumnitrit reinst
152 106600 Natriumsalicylat krist
153 106619 Brenztraubensäure-Na.-Salz f. bioch. Zwecke
154 106663 Di-Natriumtartrat-Dihydrat z. A.
155 106688 Natriumazid reinst
156 106756 Methyl-4-hydroxybenzoat Natriumsalz
157 106757 Methyl-4-hydroxybenzoat
158 106832 Natriumcyclamat
159 107069 Phloroglucin (1,3,5-Trihydroxybenzol)
160 107225 1,10-Phenanthrolin-Monohydrat z.A.
161 107230 Phenolphthalein
162 107256 L-Penylalanin f. b. Zw.
163 107260 Phenylsalicylat
164 107311 Pilocarpinhxdrochlorid, krist reinst
165 107427 Propyl-4-Hydroxybenzoat
166 107428 Propyl-4-hydroxybenzoat Natriumsalz
167 107434 L-Prolin f. b. Zwecke
168 107467 Procainhydrochlorid reinst
169 107549 Raffinose-Pentahydrat (Melitose)
170 107590 Resorcin reinst
171 107605 D-(-)-Ribose
172 107606 2-desoxy-D-Ribose
173 107640 Rübenzucker, Raffinade
174 107656 Lactose-Monohydrat gepulvert
175 107665 Salicin (2-O-(B-D-Glucopyranosido)-benzylalkohol)
176 107682 Seife medizinisch
177 107769 L-Serin
178 107959 Süßholzextrakt sprühgetrocknet
179 107978 Thioharnstoff
180 108035 Sulfanilamid reinst
181 108042 Saccharin Natrium
182 108085 Kaliumnatriumtartrat-Tetrahydrat krist reinst
183 108092 Kaliumantimon-(III)-oxid-Tartrat-Hemihydrat reinst
184 108170 Thioacetamid z.A.
185 108196 Tablettierhilfsmittel D
186 108197 Tablettierhilfsmittel K
187 108198 Tablettierhilfsmittel T
188 108337 D+Glucose wasserfrei

189 108346 D+Glucose Monohydrat
190 108353 Trehalose
191 108371 L-Tyrosin f. b. Zw.
192 108374 L-Tryptophan f. b. Zw.
193 108382 Tris(hydroxymethyl)-aminomethan (Trometamol)
194 108411 L-Threonin f. b. Zw.
195 108418 Titriplex III, (Ethylendinitrilotetraessigsäure Dinatriumsalz Dihydrat)
196 108439 Calcium-Titriplex Dihydrat
197 108484 Harnstoff, Perlform reinst
198 108486 Harnstoff reinst krist
199 108495 L-Valin
200 108510 Vanillin, Lebensmittelqual.
201 108865 Zinkstearat
202 110110 2-[4-(2-Hydroxyethyl)-1-piperazinyl]-ethansulfonsäure
203 110220 Piperazin-1,4-bis(ethansulfonsäure)
204 110550 Creatinphosphorsäure Dinatriumsalz-Tetrahydrat
205 110783 Di-Lithiumtetraborat (Spectromelt A 10)
206 110887 Dichlorisocyanursäure Natriumsalz Dihydrat
207 111037 Trinatriumcitrat
208 111352 Molinon Instant
209 111452 Phthaldialdehyd
210 111474 1,4-Dithiothreit
211 111685 Stärke (aus Weizen)
212 112081 S-Butyrylthiocholiniodid f. Bioch. Zwecke
213 112240 Melibiose Monohydrat
214 112422 N-Acetyl-L-cystein
215 112428 Amygdalin f. Bioch. Zwecke
216 112488 N-Acetyl-DL-tryptophan reinst endotoxiarm
217 113125 2,6-Dibromchinon-4-chlorimid (max. 30% Wasser) z.A.
218 114266 Polyvinylalkohol
219 115226 N-(2-Acetamido)-2-aminoethansulfonsäure
220 115230 3-[4-(2-Hydroxyethyl)-1-piperazinyl]-ropansulfonsäure
221 115231 2-[4-(2-Hydroxyethyl)-1-piperazinyl]-ethansulfonsäure Natriumsalz
222 115299 Dextromethorphanhydrobromid
223 115419 Cetylpalmitat
224 115940 Kristallviolett C.I. 42555
225 118304 Pentan-1-Sulfonsäurenatriumsalz
226 118305 Hexan-1-sulfonsäure Natriumsalz
227 118306 Heptan-1-sulfonsäure Natriumsalz
228 118307 Octan-1-sulfonsäure Natriumsalz
229 118308 Decan-1-sulfonsäure Natriumsalz
230 124511 1,4-Dithioerythrit für bioch. Zwekke
231 158626 Tri-Lithiumcitrat ca. 2 mol Wasser
232 159605 4-Aminophenol
233 270994 Thiaminchloridhydrochlorid
234 271436 Adenosin-5-diphosphorsäure Monokaliumsalz Dihydrat
235 277353 Photo Rex
236 278343 Dextroseandydrid
237 450890 Saponin
238 451318 DL-Methionin
239 458038 Ethylcellulose
240 458162 Aerosol OT
241 458268 Saponin
242 500010 Folsäure rein
243 500013 Rutin (Rutosid)
244 500090 L(+)-Ascorbylpalmitat
245 500115 Cholinhydrogentartrat, Lebensmittelqualität
246 500117 Cholinchlorid reinst
247 500157 Calcium-D(+)-Pantothenat
248 500190 Glycin krist
249 500224 Pyridoxolhydrochlorid
250 500257 Riboflavin
251 500259 Riboflavin-5-phosphat Mononatriumsalz Dihydrat
252 500297 Nicotinsäureamid
253 500675 Thiamindisulfid
254 500724 Vitamin A-acetat Trockenpulver
255 500859 Vitamin E-Trockenpulver (50g DL-A-Tocopherolacetat in 100g Substanz)
256 500980 Thiaminnitrat (Vitamin B1 Mononitrat)
257 501260 Pyridoxol
258 501551 Vitamin D3-Trockenpulver
259 501606 D+Biotin-konz. 2% gespr.
260 501902 Trihydroxyethylrutin
261 524950 Vitamin B12
262 820927 Octansäure Natriumsalz
263 907327 Piperazin-Hexahydrat

7.3 Validierungsreports

NIR (Standardmethode, Vektornormierung und 1.Ableitung)

```
Method file:                            E:\IDLIB\IP1\KL1\MTHD3\SND19d.FAA
from (date):                             4/ 1/99
     (time):                            19:11:4
Algorithm:                              Standard
For Threshold Individual:               Nein
No. of used factor sp.:                 -
For Threshold Info Entry:               1
No. of Hits to be Listed:               10
Vector normalized spectra:              Ja
No. of Spectra:                         263
Delta x of x raster:                    3.857
FXV (or LXV) mod Delta x:               7.4607e-014
min x of x raster:                      3999.71
max. x of x raster:                      11999.1
Whole x range:                          Ja
Nr. of x Points in all x Ranges:        2075
X-Ranges:                               1
From:                                   3999.71
  to:                                   11999.1
  Weight:                               1
  Reprolevel:                           1
BlockID:                                4111
Order of Derivative:                    0
Description:
For Threshold Info Entry:               TEXT:Compound Name
Path of origin reference spectra:       E:\EINZEL\KL1
Smoothing points:                       1
Method Released:                        0
Order of Internal Derivation:           1
Smoothing Points for Internal Derivation: 9
Reduction Factor:                       1
Use Thresh. From Info:                  Nein
Use Thresh. From Info Entry:            1
Use Thresh. From Info Entry:            TEXT:Compound Name


Check Average Spectra
=====================

Constant conf. level : Fixed algorithm,   Single Sphere Method
-------------------------------------------------------------
Confidence Region = 2 x Threshold

Spectra, which can be confused with other references:

File Name       Sample Name                                 Confidence Region
 100242.1        100242 | Citronensäure Monohydr             1.004088
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 100243.1        100243 | Citronensäure Monohydr   0.925198   0.503104
 100802.1        100802 | L+Weinsäure krist | Av   0.947264   0.587235
 104219.1        104219 | Guanidiniumchlorid f.    0.963606   0.220449
 105099.1        105099 | Di-Kaliumhydrogenphosp   0.906586   0.484008
 907327.1        907327 | Piperazin-Hexahydrat |   0.937345   1.040533

File Name       Sample Name                                 Confidence Region
 101124.1        101124 | Ammoniumdihydrogenphos             0.758398
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 101131.1        101131 | Ammoniumhydrogencarbon   0.680011   0.773526

File Name       Sample Name                                 Confidence Region
 101131.1        101131 | Ammoniumhydrogencarbon             0.773526
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 101124.1        101124 | Ammoniumdihydrogenphos   0.680011   0.758398
 101218.1        101218 | di-Ammoniumhydrogenpho   0.670188   0.956888
```

```
File Name       Sample Name                                  Confidence Region
 101187.1        101187 | Ammoniumnitrat reinst               0.391632
-------------------------------------------------------------------------------
       Overlapping with:                          Hit
 101211.1        101211 | Ammoniumsulfat f. b. Z   0.251700   0.448471

File Name       Sample Name                                  Confidence Region
101200.1        101200 | Ammoniumperoxodisulfat              0.471006
-------------------------------------------------------------------------------
       Overlapping with:                          Hit
 101187.1        101187 | Ammoniumnitrat reinst    0.420118   0.391632
 101211.1        101211 | Ammoniumsulfat f. b. Z   0.461298   0.448471

   File Name       Sample Name                                     Confidence Region
 101208.1        101208 | Ammoniumthiosulfat  LA               0.532495
-------------------------------------------------------------------------------
       Overlapping with:                          Hit
 101211.1        101211 | Ammoniumsulfat f. b. Z   0.521505   0.448471

File Name       Sample Name                                  Confidence Region
 101211.1        101211 | Ammoniumsulfat f. b. Z               0.448471
-------------------------------------------------------------------------------
       Overlapping with:                          Hit
 101187.1        101187 | Ammoniumnitrat reinst    0.251700   0.391632

File Name       Sample Name                                  Confidence Region
 101218.1        101218 | di-Ammoniumhydrogenpho               0.956888
-------------------------------------------------------------------------------
       Overlapping with:                          Hit
 100807.1        100807 | Trichloressigsäure | A   0.858144   0.624967
 101124.1        101124 | Ammoniumdihydrogenphos   0.884729   0.758398
 101131.1        101131 | Ammoniumhydrogencarbon   0.670188   0.773526
103767.1        103767 | Ammoniumformiat reinst   0.884624   0.539182

File Name       Sample Name                                  Confidence Region
101407.1        101407 | Kristallviolett C.I. 42              0.704777
-------------------------------------------------------------------------------
       Overlapping with:                          Hit
115940.1        115940 | Kristallviolett C.I. 42   0.028305   0.333492

File Name       Sample Name                                  Confidence Region
 102072.1        102072 | Calciumchlorid-Hexahyd               1.134704
-------------------------------------------------------------------------------
       Overlapping with:                          Hit
 100492.1        100492 | Oxalsäure-Dihydrat rei   0.878870   0.396618
100623.1        100623 | Pikrinsäure z.A. (0,5m   1.131745   0.350166
 101719.1        101719 | Bariumchlorid-Dihydrat   1.126216   0.314242
 102127.1        102127 | Beta-Cyclodextrin | Av   1.109518   0.288776
 102144.1        102144 | Calciumhydrogenphospha   1.074647   0.531808
 103006.1        103006 | Dextrin weiß | Av. of   1.118213   0.090826
 103883.1        103883 | Eisen-III-nitratNonahy   1.074546   0.210122
 104228.1        104228 | Gummi Arabisch, sprühg   1.110395   0.099201
 104982.1        104982 | Kaliumhexacyanoferrat-   1.123569   0.476212
 105099.1        105099 | Di-Kaliumhydrogenphosp   1.104069   0.484008
 105924.1        105924 | Mangan-II-carbonat-Hyd   1.102652   0.238062
 106346.1        106346 | Natriumdihydrogenphosp   1.040737   0.618181
 108484.1        108484 | Harnstoff, Perlform re   1.110541   0.174455
 501606.1        501606 D+Biotin-konz. 2% gespr.   1.121857   0.147494
 907327.1        907327 | Piperazin-Hexahydrat |   1.053368   1.040533

File Name       Sample Name                                  Confidence Region
 104350.1        104350 | L-Histidinmonohydrochl               1.037221
-------------------------------------------------------------------------------
       Overlapping with:                          Hit
 524950.1        524950 | Vitamin B12 | Av. of 1   0.984871   0.462871

File Name       Sample Name                                  Confidence Region
 105700.1        105700 | L-Lysinmonohydrochlori               0.912729
-------------------------------------------------------------------------------
       Overlapping with:                          Hit
 108495.1        108495 | L-Valin | Av. of 12      0.832032   0.220122

File Name       Sample Name                                  Confidence Region
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 105995.1        105995 | (-)-Menthol krist | Av             0.922771
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 102166.1        102166 | D(-)-Campher raffinier   0.894854   0.590237
 103672.1        103672 | Colesterin gepulvert |   0.786379   0.068346
 115419.1        115419 | Cetylpalmitat | Av. of   0.898198   0.847277
 118304.1        118304 | Pentan-1-Sulfonsäurena   0.917566   0.579100
 458162.1        458162 | Aerosol OT | Av. of  7   0.801861   0.650112
 500859.1        500859 | Vitamin E-Trockenpulve   0.905776   0.069755

File Name       Sample Name                                    Confidence Region
 106432.1        106432 | Tri-Natriumcitrat-Dihy             0.220126
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 106446.1        106446 | tri-Natriumcitrat Dihy   0.068439   0.156468

File Name       Sample Name                                    Confidence Region
 106446.1        106446 | tri-Natriumcitrat Dihy             0.156468
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 106432.1        106432 | Tri-Natriumcitrat-Dihy   0.068439   0.220126

File Name       Sample Name                                    Confidence Region
 107428.1        107428 | Propyl-4-hydroxybenzoa             0.979749
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 100886.1        100886 | Ethyl-4-hydroxybenzoat   0.813607   0.309095
 107427.1        107427 | Propyl-4-Hydroxybenzoa   0.877347   0.205656
 458038.1        458038 | Ethylcellulose | Av. o   0.924451   0.138814

File Name       Sample Name                                    Confidence Region
 107682.1        107682 | Seife medizinisch | Av             0.265627
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 105876.1        105876 | Magnesiumstearat gefäl   0.247753   0.080412

File Name       Sample Name                                    Confidence Region
 111352.1        111352 | Molinon Instant | Av.             0.635889
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 458268.1        458268 | Saponin | Av. of  5      0.607193   0.393725

File Name       Sample Name                                    Confidence Region
 111685.1        111685 | Stärke (aus Weizen) |             0.106977
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 103006.1        103006 | Dextrin weiß | Av. of    0.099303   0.090826

File Name       Sample Name                                    Confidence Region
 115419.1        115419 | Cetylpalmitat | Av. of             0.847277
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 100989.1        100989 | Cetylalkohol (1-Hexade   0.702835   0.391486
 458162.1        458162 | Aerosol OT | Av. of  7   0.819149   0.650112

File Name       Sample Name                                    Confidence Region
 115940.1        115940 | Kristallviolet C.I. 42             0.333492
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 101407.1        101407 | Kristallviolet C.I. 42   0.028305   0.704777

File Name       Sample Name                                    Confidence Region
 118304.1        118304 | Pentan-1-Sulfonsäurena             0.579100
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 118305.1        118305 | Hexan-1-sulfonsäure Na   0.396403   0.583429
 118306.1        118306 | Heptan-1-sulfonsäure N   0.467386   0.459277

File Name       Sample Name                                    Confidence Region
 118305.1        118305 | Hexan-1-sulfonsäure Na             0.583429
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 118304.1        118304 | Pentan-1-Sulfonsäurena   0.396403   0.579100
 118306.1        118306 | Heptan-1-sulfonsäure N   0.242794   0.459277
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 118307.1        118307 | Octan-1-sulfonsäure Na   0.464148   0.521464

File Name       Sample Name                                   Confidence Region
 118306.1        118306 | Heptan-1-sulfonsäure N              0.459277
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 118305.1        118305 | Hexan-1-sulfonsäure Na   0.242794   0.583429
 118307.1        118307 | Octan-1-sulfonsäure Na   0.297615   0.521464

File Name       Sample Name                                   Confidence Region
 118307.1        118307 | Octan-1-sulfonsäure Na              0.521464
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 118305.1        118305 | Hexan-1-sulfonsäure Na   0.464148   0.583429
 118306.1        118306 | Heptan-1-sulfonsäure N   0.297615   0.459277
 118308.1        118308 | Decan-1-sulfonsäure Na   0.317593   0.333075

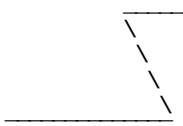
File Name       Sample Name                                   Confidence Region
 118308.1        118308 | Decan-1-sulfonsäure Na              0.333075
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 118307.1        118307 | Octan-1-sulfonsäure Na   0.317593   0.521464

File Name       Sample Name                                   Confidence Region
 450890.1        450890 | Saponin | Av. of  9                0.289127
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 107656.1        107656 | Lactose-Monohydrat gep   0.203503   0.045294
 501551.1        501551 | Vitamin D3-Trockenpulv   0.174995   0.453883

File Name       Sample Name                                   Confidence Region
 501551.1        501551 | Vitamin D3-Trockenpulv              0.453883
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 107656.1        107656 | Lactose-Monohydrat gep   0.253547   0.045294
 450890.1        450890 | Saponin | Av. of  9      0.174995   0.289127

File Name       Sample Name                                   Confidence Region
 907327.1        907327 | Piperazin-Hexahydrat |              1.040533
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 100242.1        100242 | Citronensäure Monohydr   0.937345   1.004088
 100492.1        100492 | Oxalsäure-Dihydrat rei   0.961665   0.396618
 103883.1        103883 | Eisen-III-nitratNonahy   0.914132   0.210122
 105099.1        105099 | Di-Kaliumhydrogenphosp   0.819565   0.484008
 108484.1        108484 | Harnstoff, Perlform re   0.988493   0.174455
 108486.1        108486 | Harnstoff reinst krist   1.018105   0.298561

Summary:
--------
Average Spectra, which can be confused with other references:   29 of 263
Average Spectra, which can be uniquely identified:   234 of 263
 100010.1        100010 | Acetanilid reinst kris
 100085.1        100085 | Acetylsalicylsäure | A
 100090.1        451552 | Adipinsäure reinst | A
 100102.1        100102 | 4-Aminobenzuesäure rei
 100103.1        100103 | Amidoschwefelsäure z.A
 100126.1        100126 | L-Asparaginsäure für b
 100130.1        100130 | Benzoesäure gepulvert
 100138.1        100138 | 3,5-Dinitrobenzoesäure
 100162.1        100162 | Borsäure gepulvert rei
 100163.1        100163 | Di-Bortrioxid | Av. of
```



Raman (Standardmethode, Vektornormierung und 1.Ableitung)

```
Method file:                            D:\IDLIB\IP1\KL2\MTHD3\SND19c.FAA
from (date):                             5/ 1/99
     (time):                            15: 2:48
Algorithm:                              Standard
For Threshold Individual:               Nein
No. of used factor sp.:                 -
For Threshold Info Entry:               1
No. of Hits to be Listed:               10
Vector normalized spectra:              Ja
No. of Spectra:                         263
Delta x of x raster:                    0.96425
FXV (or LXV) mod Delta x:               0.280662
min x of x raster:                      99.5984
max x of x raster:                      3499.54
Whole x range:                          Ja
No. of x Points in all x Ranges:        3527
X-Ranges:                               1
From:                                   99.5984
  to:                                   3499.54
  Weight:                               1
  Reprolevel:                           1
BlockID:                                10255
Order of Derivative:                    0
Description:
For Threshold Info Entry:
Path of origin reference spectra:       D:\EINZEL\KL21
Smoothing points:                       1
Method Released:                        0
Order of Internal Derivation:           1
Smoothing Points for Internal Derivation: 9
Reduction Factor:                       1
Use Thresh. From Info:                  Nein
Use Thresh. From Info Entry:            1
Use Thresh. From Info Entry:


Check Average Spectra
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Constant conf. level : Fixed algorithm,   Single Sphere Method
-----------------------------------------------------------------
Confidence Region = 2 x Threshold

Spectra, which can be confused with other references:

File Name       Sample Name                                 Confidence Region
 100242.1        100242 | Citronens„ure Monohydr             0.458916
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 100243.1        100243 | Citronens„ure Monohydr   0.093363   0.544981

File Name       Sample Name                                 Confidence Region
 100243.1        100243 | Citronens„ure Monohydr             0.544981
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 100242.1        100242 | Citronens„ure Monohydr   0.093363   0.458916

File Name       Sample Name                                 Confidence Region
 100989.1        100989 | Cetylalkohol (1-Hexade             0.589218
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 100671.1        100671 | Stearins„ure | Av. of    0.298740   0.026060
 101107.1        101107 | Aluminiumstearat | Av.   0.405257   0.075229
 102154.1        102154 | Calciumstearat | Av. o   0.424873   0.107628
 105876.1        105876 | Magnesiumstearat gef„l   0.431600   0.123470
 107682.1        107682 | Seife medizinisch | Av   0.494031   0.123429
 108865.1        108865 | Zinkstearat | Av. of     0.486698   0.029438
 115419.1        115419 | Cetylpalmitat | Av. of   0.230904   0.147221
 118308.1        118308 | Decan-1-sulfons„ure Na   0.504881   0.666383
 500090.1        500090 | L(+)-Ascorbylpalmitat    0.429206   0.084882
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File Name       Sample Name                                  Confidence Region
 101407.1        101407 | Kristallviolet C.I. 42              0.980783
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 115940.1        115940 | Kristallviolet C.I. 42    0.017617   0.308797

File Name       Sample Name                                  Confidence Region
 102070.1        102070 | Calciumchlorid 90-95%               1.354308
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 100492.1        100492 | Oxals„ure-Dihydrat rei    1.321093   0.192883
 100807.1        100807 | Trichloressigs„ure | A    1.308760   0.217889
 100963.1        100963 | DL-Alanin f•r bioch. Z    1.351249   0.047640
 101190.1        101190 | Di-Ammoniumoxalat-Mono    1.354168   0.222898
 101226.1        101226 | Ammoniummonovanadat z.    1.352215   0.034159
 102146.1        102146 | Calciumhydrogenphospha    1.350569   0.221331
 102148.1        102148 | Calcium-D-Saccharat re    1.341081   0.138641
 102851.1        102851 | Calciumlaevulinat rein    1.329423   0.096867
 104128.1        104128 | Auxillin (Gibberillin     1.311841   0.142809
 104350.1        104350 | L-Histidinmonohydrochl    1.177595   0.415788
 106467.1        106467 | Natriumhydroxi granuli    1.038939   0.417924
 106544.1        106544 | Natriumnitrit reinst |    1.295365   0.205559
 107959.1        107959 | S•áholzextrakt spr•hge    1.311896   3.519427
 108371.1        108371 | L-Tyrosin f. b. Zw. |     1.246063   0.173634
 112428.1        112428 | Amygdalin f. Bioch. Zw    1.292664   0.969447
 159605.1        159605 | 4-Aminophenol | Av. of    1.265652   0.043963
 271436.1        271436 | Adenosin-5-diphosphors    1.351799   0.178478

File Name       Sample Name                                  Confidence Region
 102072.1        102072 | Calciumchlorid-Hexahyd            1.431255
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 100010.1        100010 | Acetanilid reinst kris    1.288162   0.082312
 100085.1        100085 | Acetylsalicyls„ure | A    1.320809   0.055139
 100090.1        100090 | Adipins„ure reinst | A    1.402201   0.044166
 100102.1        100102 | 4-Aminobenzues„ure rei    1.425541   0.070165
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File Name       Sample Name                                  Confidence Region
 102127.1        102127 | Beta-Cyclodextrin | Av            0.807182
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 103006.1        103006 | Dextrin weiá | Av. of    0.514819   0.147478
 111685.1        111685 | St„rke (aus Weizen) |    0.516588   0.168958
 501606.1        501606 | D+Biotin-konz. 2% gesp   0.598752   0.194068

File Name       Sample Name                                  Confidence Region
 102530.1        102530 | Cobalt-II-acetat Tetra            1.291127
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 103962.1        103962 | Eisen(II)-fumarat, rei    0.311091   0.336673
 107959.1        107959 | S•áholzextrakt spr•hge    1.249914   3.519427

File Name       Sample Name                                  Confidence Region
 103006.1        103006 | Dextrin weiá | Av. of            0.147478
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 111685.1        111685 | St„rke (aus Weizen) |    0.130752   0.168958

File Name       Sample Name                                  Confidence Region
 103962.1        103962 | Eisen(II)-fumarat, rei            0.336673
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
 102530.1        102530 | Cobalt-II-acetat Tetra   0.311091   1.291127

File Name       Sample Name                                  Confidence Region
 104168.1        104168 | Beta-Glycerophosphat D            1.094834
-------------------------------------------------------------------------------
       Overlapping with:                             Hit
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 102146.1        102146 | Calciumhydrogenphospha   0.880818   0.221331
 110550.1        110550 | Creatinphosphors„ure D   1.047801   0.716645

File Name       Sample Name                                  Confidence Region
 104349.1        104349 | Homatropinmethylbromid              1.304249
-------------------------------------------------------------------------------
       Overlapping with:                              Hit
 100010.1        100010 | Acetanilid reinst kris   1.144573   0.082312
 100102.1        100102 | 4-Aminobenzues„ure rei   1.296015   0.070165
 100126.1        100129 | L-Asparagins„ure reins   1.219044   0.092033
 100130.1        100130 | Benzoes„ure gepulvert    1.090488   0.055978
 100289.1        100289 | L-Glutamin f. bioch. Z   1.217203   0.176502
 101155.1        101155 | Di-Ammoniumhydrogencit   1.300302   0.818903
 101838.1        101838 | Curco BS | Av. of  6    1.237595   0.155954
 102166.1        102166 | D(-)-Campher raffinier   1.279589   0.073816
 102424.1        102424 | Chloramin T Trihydrat    1.252674   0.394545
 102425.1        102425 | Chloralhydrat | Av. of   1.265094   0.084440
 102584.1        102584 | Coffein rein | Av. of    1.207450   0.080836
 102838.1        102838 | L-Cystein f•r bioch. Z   1.199320   0.241116
 103149.1        103149 | (+-)-Ephedrinhydrochlo   1.109581   0.090064
 104343.1        104343 | Methenamin | Av. of  8   1.101072   0.097719
 104506.1        104506 | L-Hydroxyprolin f. b.    1.036860   3.085978
 105995.1        105995 | (-)-Menthol krist | Av   1.302672   0.949150
 106129.1        106129 | 3-Morpholinopropansulf   1.209550   0.161772
 107069.1        107069 | Phloroglucin (1,3,5-Tr   1.235970   0.281414
 107230.1        107230 | Phenolphthalein | Av.    1.265307   0.102357
 107256.1        107256 | L-Penylalanin f. b. Zw   1.075289   0.084684
 107260.1        107260 | Phenylsalicylat | Av.    1.255347   0.107905
 107590.1        107590 | Resorcin reinst | Av.    1.272124   0.114703
 107606.1        107606 | 2-desoxy-D-Ribose | Av   1.183087   0.089816
 107769.1        107769 | L-Serin | Av. of  8      1.204478   0.162600
 110220.1        110220 | Piperazin-1,4-bis(etha   1.295696   0.691588
 111037.1        111037 | Trinatriumcitrat | Av.   1.271296   0.158675
 112428.1        112428 | Amygdalin f. Bioch. Zw   1.095353   0.969447
 115230.1        115230 | 3-[4-(2-Hydroxyethyl)-   1.187180   0.157989
 907327.1        907327 | Piperazin-Hexahydrat |   1.272478   0.703618

File Name       Sample Name                                  Confidence Region
 104506.1        104506 | L-Hydroxyprolin f. b.               3.085978
-------------------------------------------------------------------------------
       Overlapping with:                              Hit
 100010.1        100010 | Acetanilid reinst kris   1.435668   0.082312
 100085.1        100085 | Acetylsalicyls„ure | A   1.467487   0.055139
 100090.1        100090 | Adipins„ure reinst | A   1.491228   0.044166
 100102.1        100102 | 4-Aminobenzues„ure rei   1.365937   0.070165
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File Name       Sample Name                                  Confidence Region
 105072.1        105072 | Di-Kaliumoxalat-Monohy            3.055652
-------------------------------------------------------------------------------
       Overlapping with:                              Hit
 100010.1        100010 | Acetanilid reinst kris   1.325698   0.082312
 100085.1        100085 | Acetylsalicyls„ure | A   1.354947   0.055139
 100090.1        100090 | Adipins„ure reinst | A   1.391741   0.044166
 100102.1        100102 | 4-Aminobenzues„ure rei   1.372636   0.070165
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262         \
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File Name       Sample Name                                  Confidence Region
 105102.1        105102 | Tri-Kaliumphosphat-Tri            0.683779
-------------------------------------------------------------------------------
       Overlapping with:                              Hit
 101124.1        101124 | Ammoniumdihydrogenphos   0.593942   0.207669

File Name       Sample Name                                  Confidence Region
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 105700.1       105700 | L-Lysinmonohydrochlori             1.397607
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 100103.1       100103 | Amidoschwefels„ure z.A   1.322880   0.046911
 100126.1       100129 | L-Asparagins„ure reins   1.348678   0.092033
 100138.1       100138 | 3,5-Dinitrobenzoes„ure   1.393947   0.032759
 100242.1       100242 | Citronens„ure Monohydr   1.368592   0.458916
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File Name       Sample Name                                 Confidence Region
 105870.1       105870 | Magnesiumhydroxid, rei             3.057661
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 100010.1       100010 | Acetanilid reinst kris   1.411926   0.082312
 100085.1       100085 | Acetylsalicyls„ure | A   1.411502   0.055139
 100090.1       100090 | Adipins„ure reinst | A   1.414443   0.044166
 100102.1       100102 | 4-Aminobenzues„ure rei   1.412764   0.070165

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File Name       Sample Name                                 Confidence Region
 105876.1       105876 | Magnesiumstearat gef„l             0.123470
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 101107.1       101107 | Aluminiumstearat | Av.   0.103617   0.075229

File Name       Sample Name                                 Confidence Region
 105924.1       105924 | Mangan-II-carbonat-Hyd             0.761684
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 102071.1       102071 | Calciumcarbonat f. op.   0.661065   0.011004

File Name       Sample Name                                 Confidence Region
 105995.1       105995 | (-)-Menthol krist | Av             0.949150
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 500859.1       500859 | Vitamin E-Trockenpulve   0.934005   0.094467

File Name       Sample Name                                 Confidence Region
 106432.1       106432 | Tri-Natriumcitrat-Dihy             0.178043
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 106446.1       106446 | tri-Natriumcitrat Dihy   0.036992   0.249648

File Name       Sample Name                                 Confidence Region
 106446.1       106446 | tri-Natriumcitrat Dihy             0.249648
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 106432.1       106432 | Tri-Natriumcitrat-Dihy   0.036992   0.178043

File Name       Sample Name                                 Confidence Region
 107428.1       107428 | Propyl-4-hydroxybenzoa             1.665151
-------------------------------------------------------------------------------------------
       Overlapping with:                              Hit
 100010.1       100010 | Acetanilid reinst kris   1.395932   0.082312
 100085.1       100085 | Acetylsalicyls„ure | A   1.464164   0.055139
 100090.1       100090 | Adipins„ure reinst | A   1.423003   0.044166
 100102.1       100102 | 4-Aminobenzues„ure rei   1.295012   0.070165
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262         \
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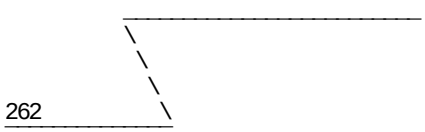
File Name       Sample Name                                 Confidence Region
 107656.1        107656 | Lactose-Monohydrat gep             0.067694
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 501551.1        501551 | Vitamin D3-Trockenpulv   0.036849   0.081402

File Name       Sample Name                                 Confidence Region
 107959.1        107959 | S•áholzextrakt spr•hge             3.519427
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 100010.1        100010 | Acetanilid reinst kris   1.414047   0.082312
 100085.1        100085 | Acetylsalicyls„ure | A   1.394373   0.055139
 100090.1        100090 | Adipins„ure reinst | A   1.414481   0.044166
 100102.1        100102 | 4-Aminobenzues„ure rei   1.418794   0.070165
```

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File Name       Sample Name                                 Confidence Region
 108198.1        108198 | Tablettierhilfsmittel T             0.559912
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 108196.1        108196 | Tablettierhilfsmittel D   0.393236   0.306419

File Name       Sample Name                                 Confidence Region
 108337.1        108337 | D+Glucose wasserfrei |              0.069033
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 278343.1        278343 | Dextroseandydrid | Av.   0.042041   0.081600

File Name       Sample Name                                 Confidence Region
 108484.1        108484 | Harnstoff, Perlform re             0.131105
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 108486.1        108486 | Harnstoff reinst krist   0.015151   0.084571

File Name       Sample Name                                 Confidence Region
 108486.1        108486 | Harnstoff reinst krist             0.084571
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 108484.1        108484 | Harnstoff, Perlform re   0.015151   0.131105

File Name       Sample Name                                 Confidence Region
 111352.1        111352 | Molinon Instant | Av.              0.695643
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 105321.1        105321 | D-(-)-Fructose reinst    0.475020   0.180837

File Name       Sample Name                                 Confidence Region
 111685.1        111685 | St„rke (aus Weizen) |              0.168958
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 103006.1        103006 | Dextrin weiá | Av. of    0.130752   0.147478

File Name       Sample Name                                 Confidence Region
 112428.1        112428 | Amygdalin f. Bioch. Zw             0.969447
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 100010.1        100010 | Acetanilid reinst kris   0.942432   0.082312
 100130.1        100130 | Benzoes„ure gepulvert    0.956024   0.055978

File Name       Sample Name                                 Confidence Region
 115940.1        115940 | Kristallviolet C.I. 42             0.308797
-------------------------------------------------------------------------------------
       Overlapping with:                            Hit
 101407.1        101407 | Kristallviolet C.I. 42   0.017617   0.980783

File Name       Sample Name                                 Confidence Region
 118305.1        118305 | Hexan-1-sulfons„ure Na             0.739253
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-------------------------------------------------------------------------------------
      Overlapping with:                          Hit
 118304.1       118304 | Pentan-1-Sulfons„urena   0.637670   0.529805
 118306.1       118306 | Heptan-1-sulfons„ure N   0.375709   0.581004

File Name      Sample Name                                   Confidence Region
 118306.1       118306 | Heptan-1-sulfons„ure N              0.581004
-------------------------------------------------------------------------------------
      Overlapping with:                          Hit
 118305.1       118305 | Hexan-1-sulfons„ure Na   0.375709   0.739253
 118307.1       118307 | Octan-1-sulfons„ure Na   0.540796   0.804557

File Name      Sample Name                                   Confidence Region
 118307.1       118307 | Octan-1-sulfons„ure Na              0.804557
-------------------------------------------------------------------------------------
      Overlapping with:                          Hit
 100671.1       100671 | Stearins„ure | Av. of    0.670867   0.026060
 100989.1       100989 | Cetylalkohol (1-Hexade   0.717941   0.589218
 101107.1       101107 | Aluminiumstearat | Av.   0.546261   0.075229
 102154.1       102154 | Calciumstearat | Av. o   0.716758   0.107628
 105876.1       105876 | Magnesiumstearat gef„l   0.534584   0.123470
 107682.1       107682 | Seife medizinisch | Av   0.547598   0.123429
 108865.1       108865 | Zinkstearat | Av. of     0.739485   0.029438
 115419.1       115419 | Cetylpalmitat | Av. of   0.626674   0.147221
 118305.1       118305 | Hexan-1-sulfons„ure Na   0.778760   0.739253
 118306.1       118306 | Heptan-1-sulfons„ure N   0.540796   0.581004
 118308.1       118308 | Decan-1-sulfons„ure Na   0.402931   0.666383
 500090.1       500090 | L(+)-Ascorbylpalmitat    0.615216   0.084882

File Name      Sample Name                                   Confidence Region
 118308.1       118308 | Decan-1-sulfons„ure Na              0.666383
-------------------------------------------------------------------------------------
      Overlapping with:                          Hit
 100671.1       100671 | Stearins„ure | Av. of    0.396762   0.026060
 100989.1       100989 | Cetylalkohol (1-Hexade   0.504881   0.589218
 101107.1       101107 | Aluminiumstearat | Av.   0.261219   0.075229
 102154.1       102154 | Calciumstearat | Av. o   0.439122   0.107628
 105876.1       105876 | Magnesiumstearat gef„l   0.248754   0.123470
 107682.1       107682 | Seife medizinisch | Av   0.460189   0.123429
 108865.1       108865 | Zinkstearat | Av. of     0.530342   0.029438
 115419.1       115419 | Cetylpalmitat | Av. of   0.385547   0.147221
 118307.1       118307 | Octan-1-sulfons„ure Na   0.402931   0.804557
 500090.1       500090 | L(+)-Ascorbylpalmitat    0.421376   0.084882

File Name      Sample Name                                   Confidence Region
 278343.1       278343 | Dextroseandydrid | Av.            0.081600
-------------------------------------------------------------------------------------
      Overlapping with:                          Hit
 108337.1       108337 | D+Glucose wasserfrei |   0.042041   0.069033

File Name      Sample Name                                   Confidence Region
 450890.1       450890 | Saponin | Av. of 10               0.131734
-------------------------------------------------------------------------------------
      Overlapping with:                          Hit
 501551.1       501551 | Vitamin D3-Trockenpulv   0.117565   0.081402

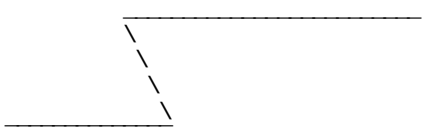
File Name      Sample Name                                   Confidence Region
 451318.1       451318 | DL-Methionin | Av. of            0.987647
-------------------------------------------------------------------------------------
      Overlapping with:                          Hit
 105707.1       105707 | L-Methionin | Av. of     0.584818   0.034623

File Name      Sample Name                                   Confidence Region
 501551.1       501551 | Vitamin D3-Trockenpulv            0.081402
-------------------------------------------------------------------------------------
      Overlapping with:                          Hit
 107656.1       107656 | Lactose-Monohydrat gep   0.036849   0.067694

File Name      Sample Name                                   Confidence Region
 102162.1       102162 | Calciumsulfat Hemihydr            1.337265
-------------------------------------------------------------------------------------
      Overlapping with:                          Hit
 101841.1       101841 | Oxals„ure-bis-(Cyclohe   1.129260   0.058678
 104005.1       104005 | Paraformaldehyd reinst   1.302986   0.051862
```

```
 107311.1        107311 | Pilocarpinhxdrochlorid   1.287550   0.092759
 501902.1        501902 | Trihydroxyethylrutin |   1.336778   0.299547
 524950.1        524950 | Vitamin B12 | Av. of 1   1.045725   0.135492


Summary:
--------
Average Spectra, which can be confused with other references:   42 of 263
Average Spectra, which can be uniquely identified:   221 of 263
 100010.1        100010 | Acetanilid reinst kris
 100085.1        100085 | Acetylsalicyls„ure | A
 100090.1        100090 | Adipins„ure reinst | A
 100102.1        100102 | 4-Aminobenzues„ure rei
 100103.1        100103 | Amidoschwefels„ure z.A
 100126.1        100129 | L-Asparagins„ure reins
 100130.1        100130 | Benzoes„ure gepulvert
 100138.1        100138 | 3,5-Dinitrobenzoes„ure
 100162.1        100162 | Bors„ure gepulvert rei
 100163.1        100163 | Di-Bortrioxid | Av. of
 100241.1        100241 | Citronens„ure wasserfr
 100289.1        100289 | L-Glutamin f. bioch. Z
 100290.1        100290 | L-Glutamins„ure reinst
```



KL2 Bin

12 100242# 13 100243 3
13 100243# 12 100242 3
21 100671# 37 101107 2
21 100671# 132 105876 3
21 100671# 223 115419 3
21 100671# 229 118308 4
33 100989# 223 115419 4
37 101107# 21 100671 2
37 101107# 70 102154 3
37 101107# 132 105876 1
37 101107# 223 115419 1
45 101187# 115 105061 4
53 101407# 224 115940 1
70 102154# 37 101107 3
70 102154# 132 105876 4
70 102154# 201 108865 2
70 102154# 223 115419 4
73 102196# 78 102530 3
73 102196# 91 103962 3
78 102530# 73 102196 3
78 102530# 114 104982 4
78 102530# 121 105125 4
78 102530# 145 106392 4
78 102530# 155 106688 4
85 103006# 211 111685 3
91 103962# 73 102196 3
91 103962# 114 104982 4
91 103962# 121 105125 4
91 103962# 145 106392 4
91 103962# 155 106688 4
114 104982# 78 102530 4
114 104982# 91 103962 4
114 104982# 145 106392 4
115 105061# 45 101187 4
115 105061# 155 106688 3
121 105125# 78 102530 4
121 105125# 91 103962 4
121 105125# 155 106688 4
127 105691# 150 106467 4
132 105876# 21 100671 3
132 105876# 37 101107 1
132 105876# 70 102154 4
132 105876# 223 115419 2
145 106392# 78 102530 4
145 106392# 91 103962 4
145 106392# 114 104982 4
147 106432# 149 106446 3
149 106446# 147 106432 3
150 106467# 127 105691 4
155 106688# 78 102530 4
155 106688# 91 103962 4
155 106688# 115 105061 3
155 106688# 121 105125 4
174 107656# 237 450890 2
174 107656# 258 501551 3
188 108337# 236 278343 4
201 108865# 70 102154 2
211 111685# 85 103006 3
223 115419# 21 100671 3
223 115419# 33 100989 4
223 115419# 37 101107 1
223 115419# 70 102154 4
223 115419# 132 105876 2
224 115940# 53 101407 1
229 118308# 21 100671 4
236 278343# 188 108337 4
237 450890# 174 107656 2
258 501551# 174 107656 3

7.4 Matrixdarstellungen

7.4.1 NIR, Standardmethode

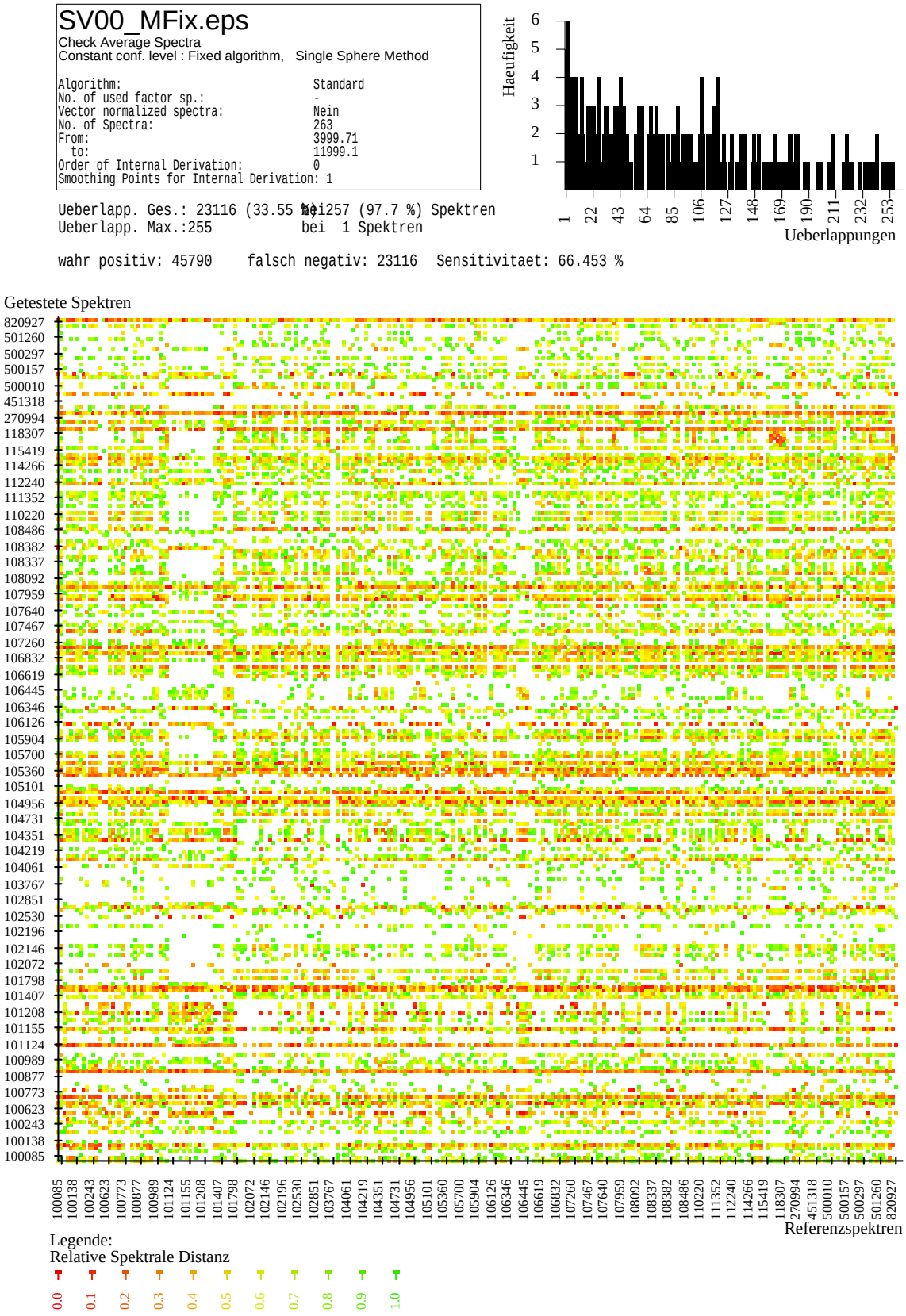


Abb. N1: Standardmethode ohne Vorbehandlung.

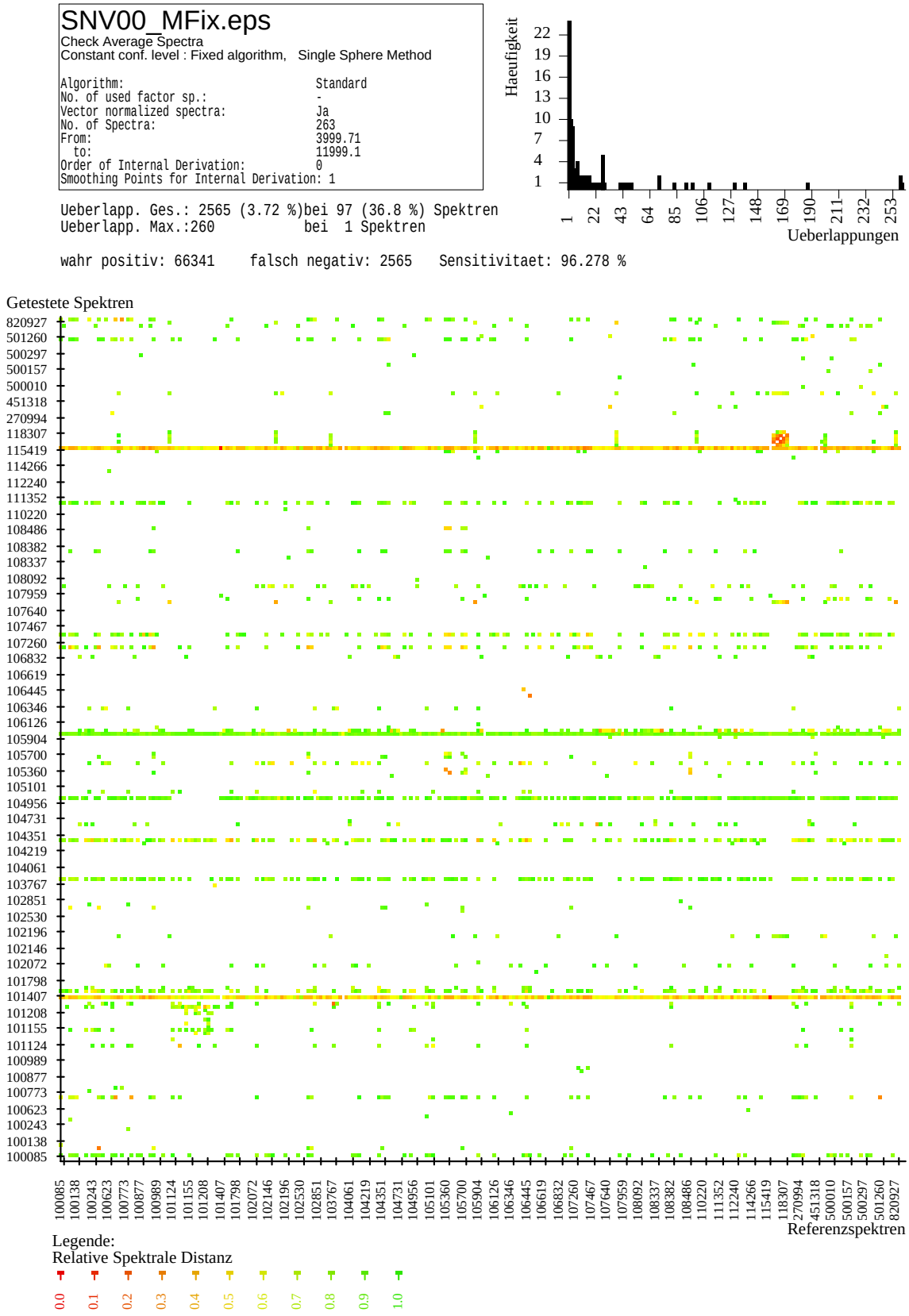


Abb. N2: Standardmethode (Vektornormierung).

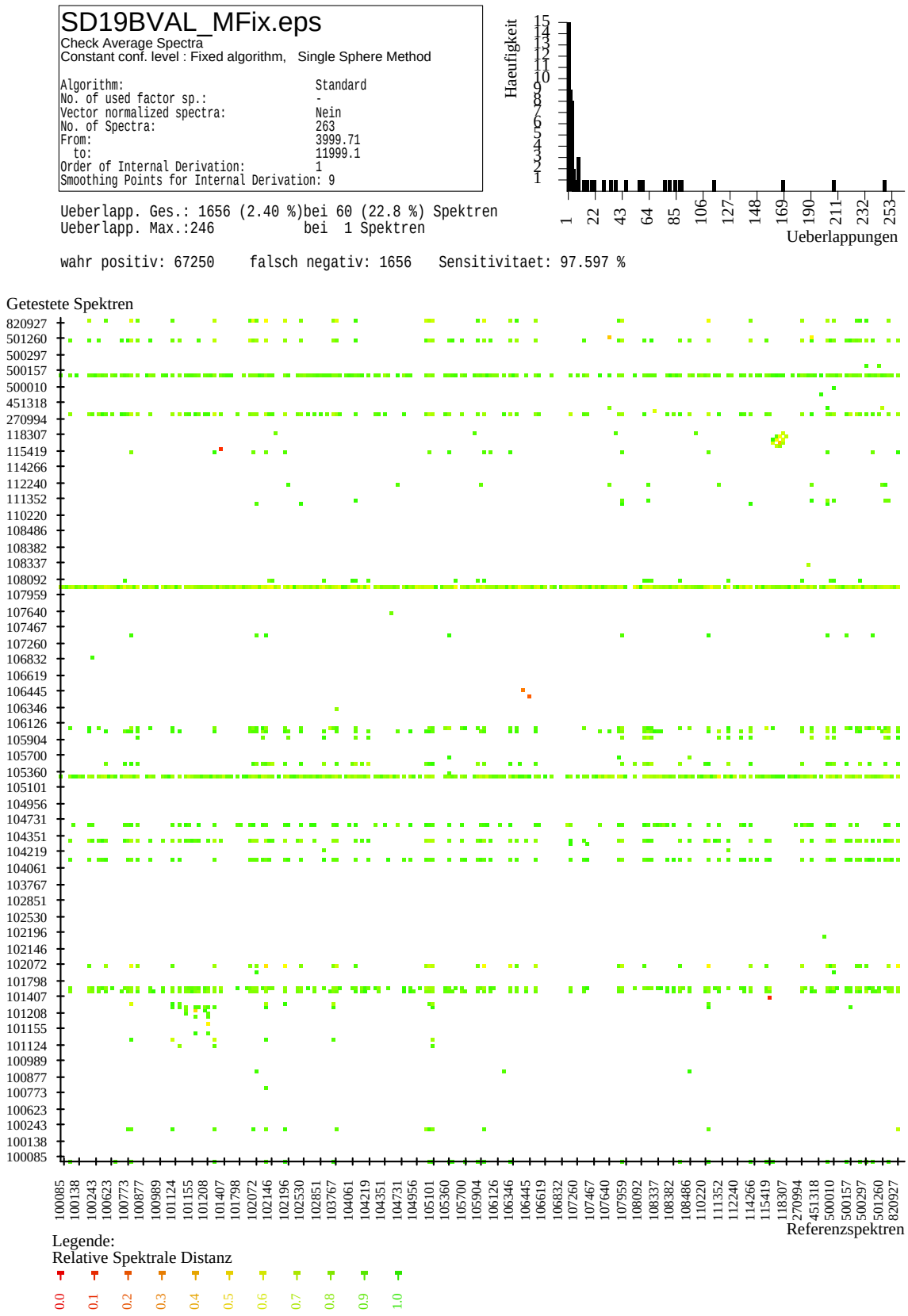


Abb. N3: Standardmethode (1. Ableitung).

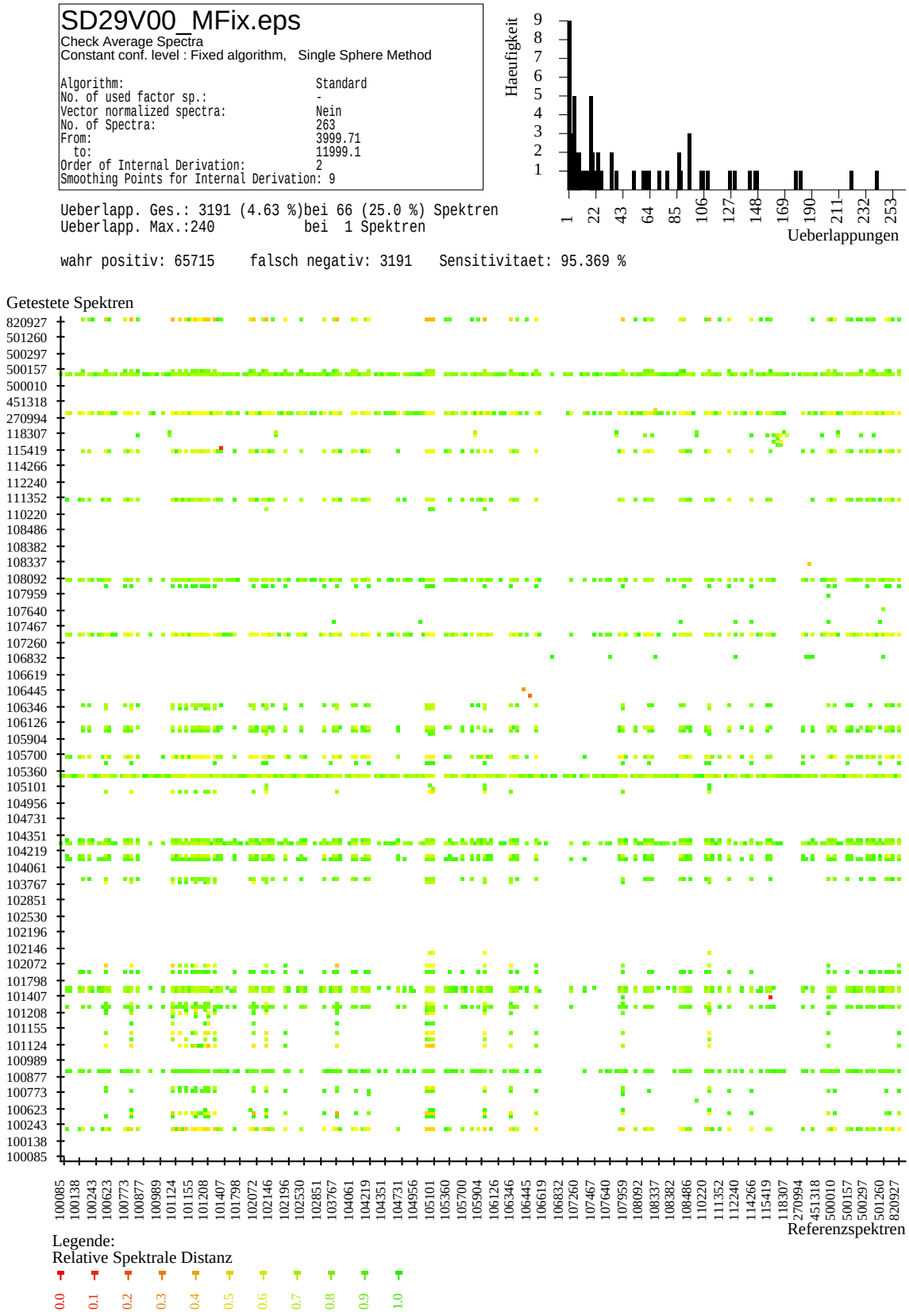


Abb. N4: Standardmethode (2. Ableitung).

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

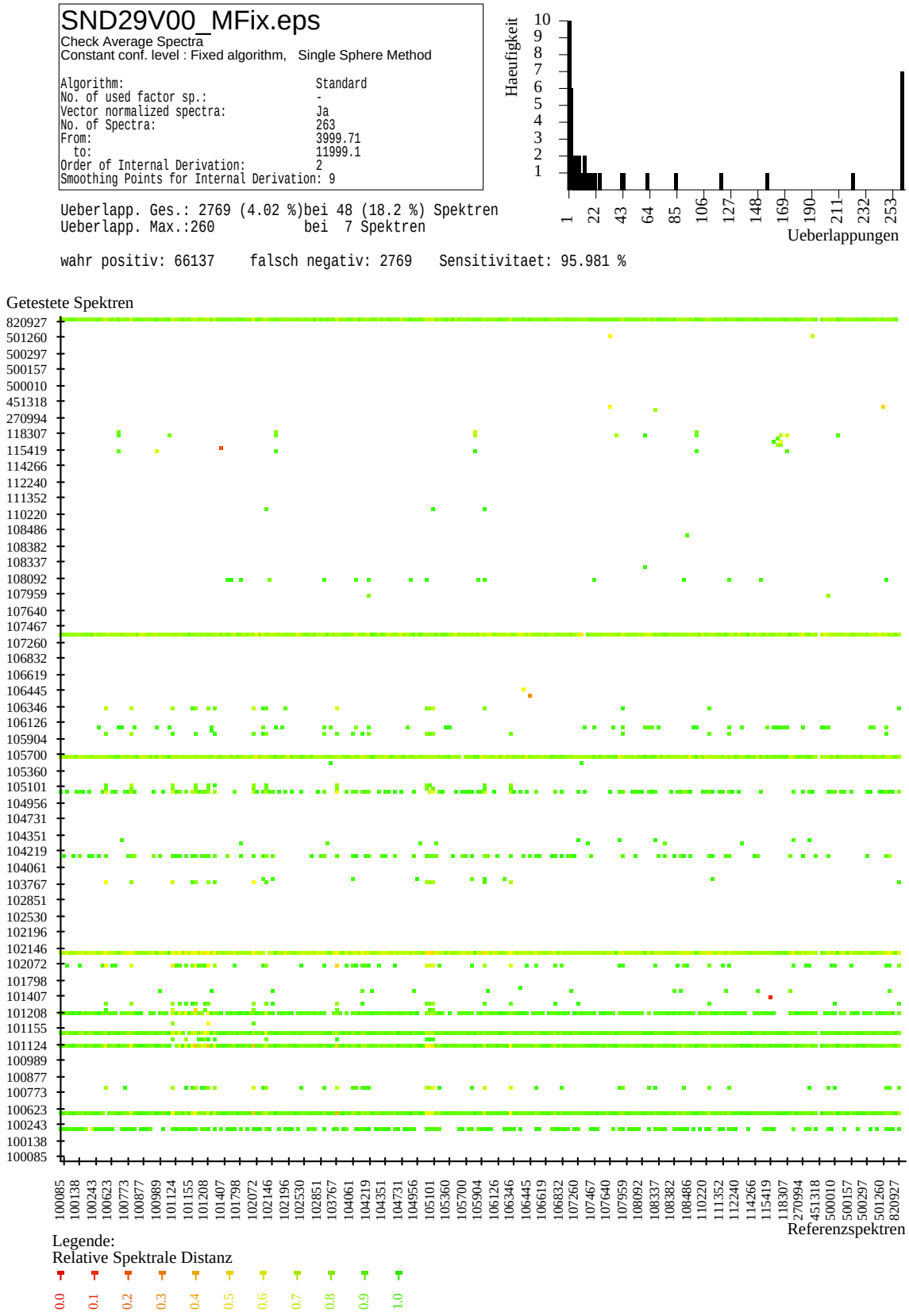


Abb. N6: Standardmethode (Vektornormierung und 2. Ableitung).

7.4.2 NIR, Faktormethode

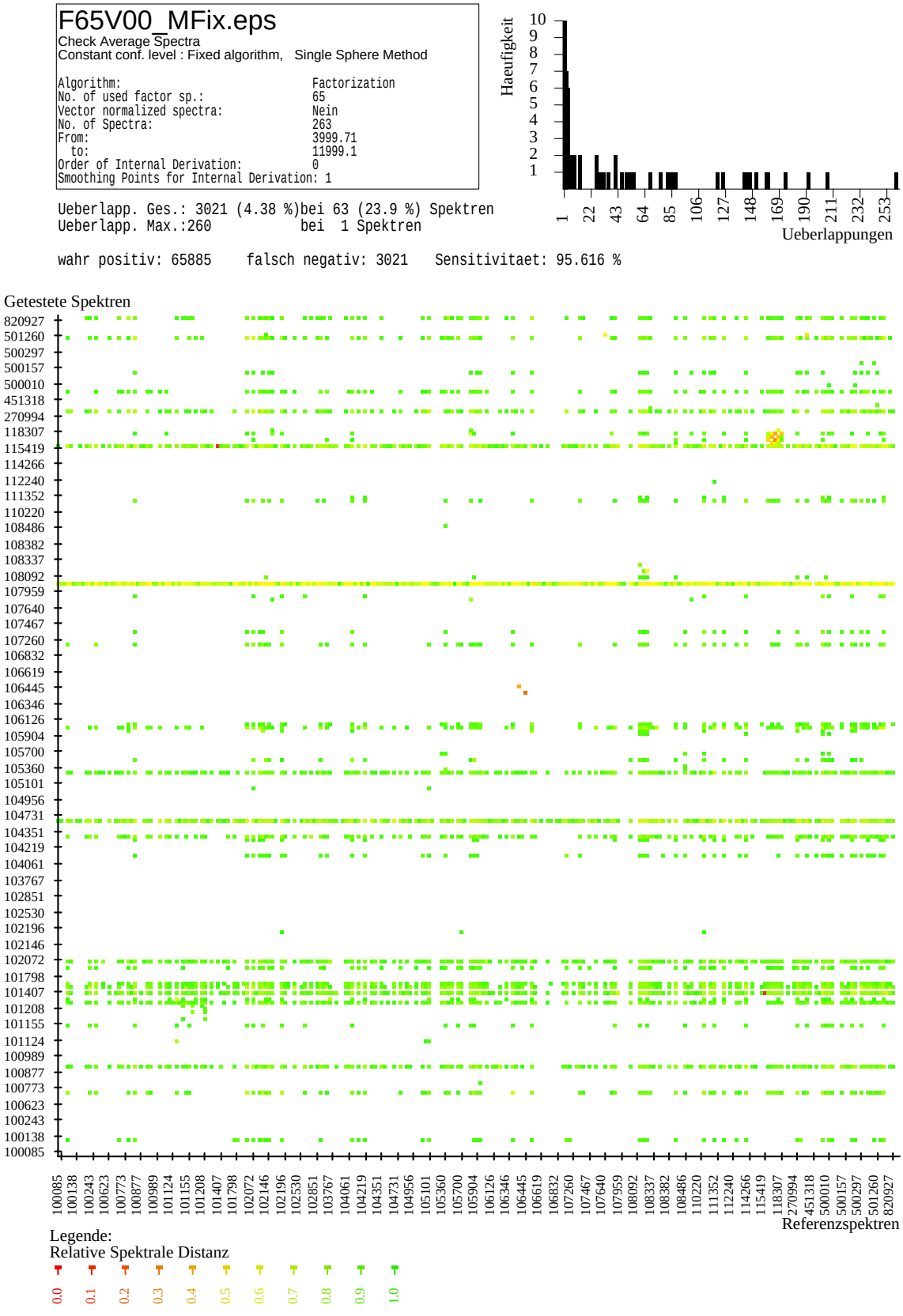


Abb. N7: Faktormethode (65 Faktoren).

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

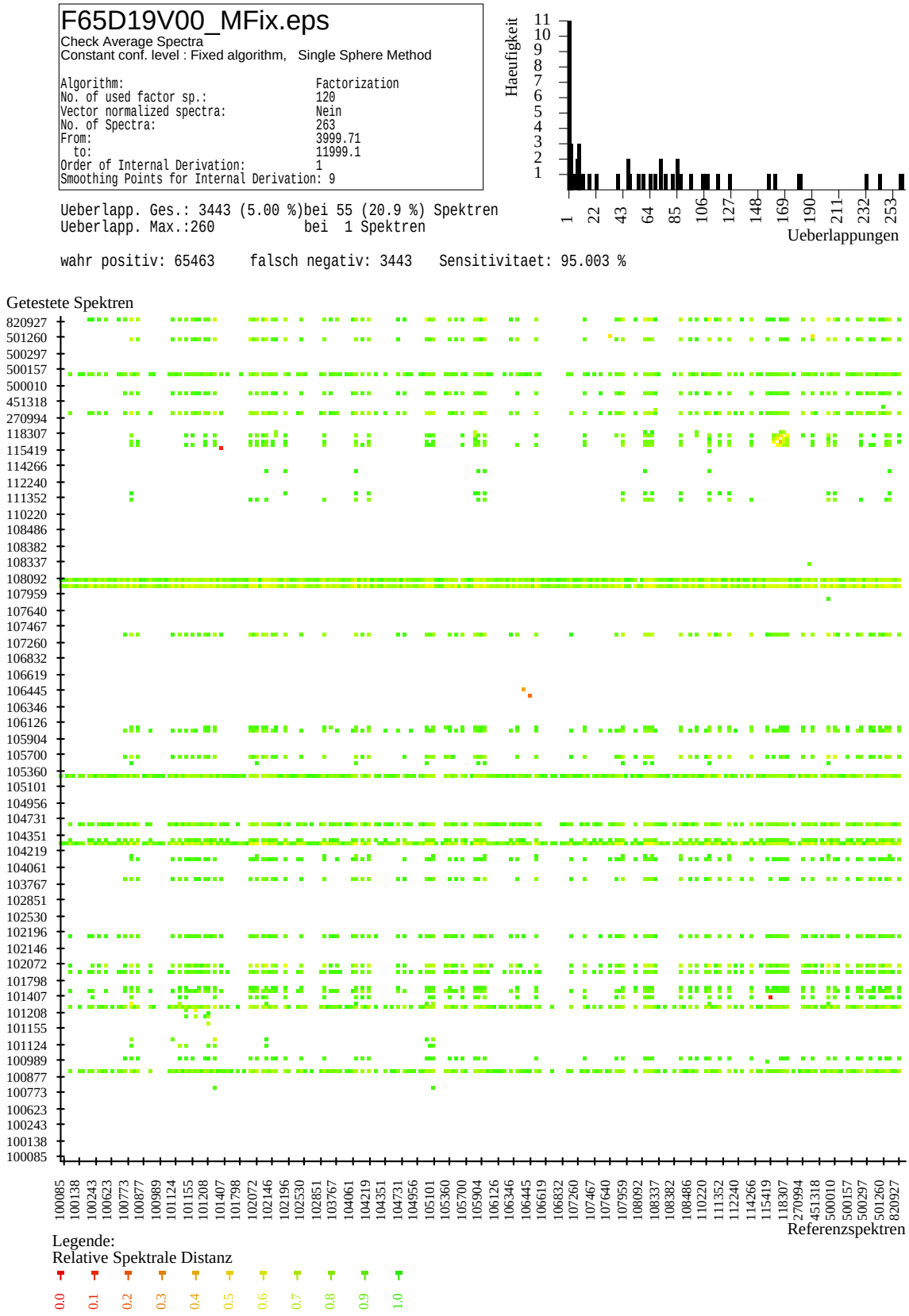


Abb. N9: Faktormethode (65 Faktoren, 1. Ableitung).

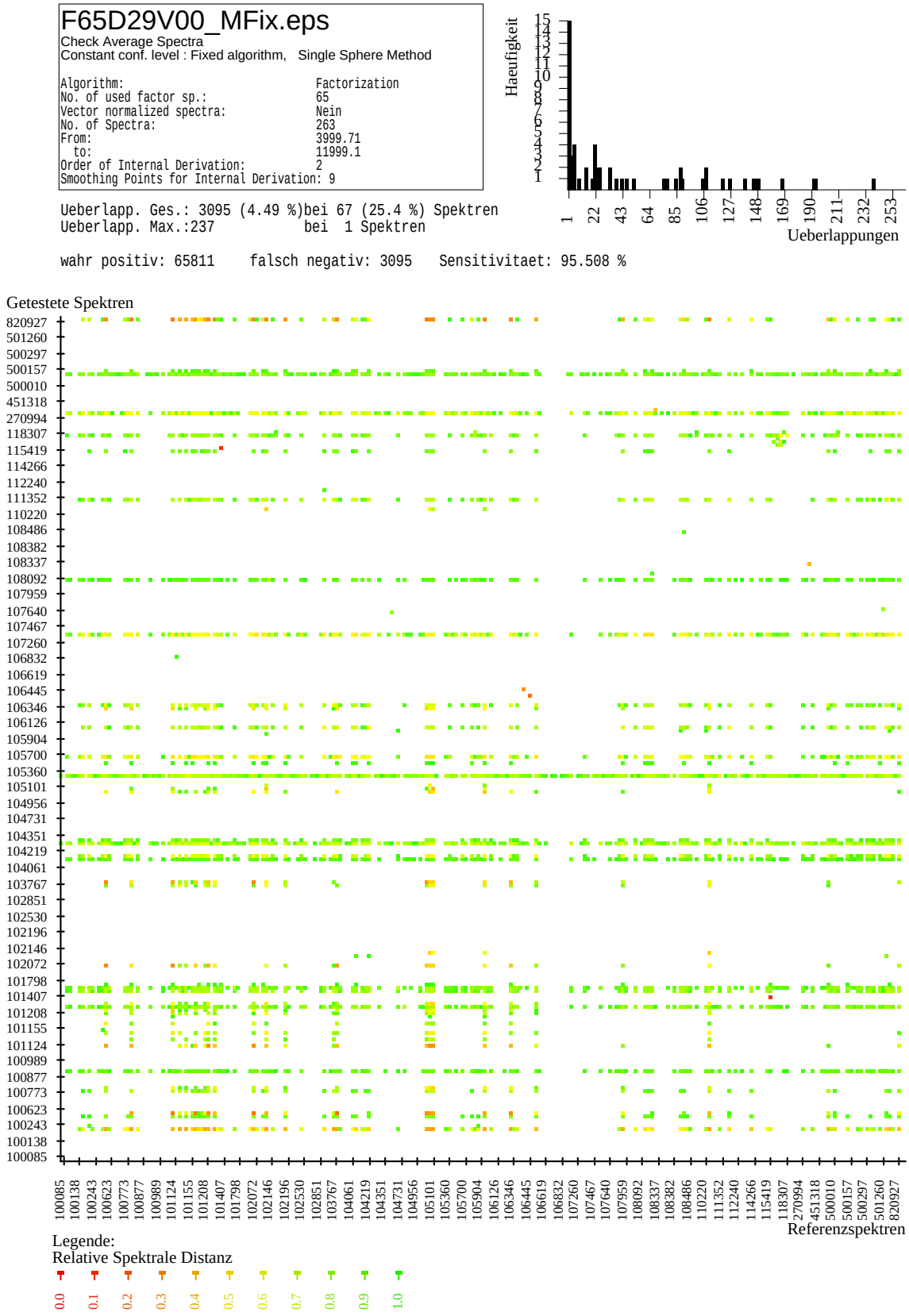


Abb. N10: Faktormethode (65 Faktoren, 2. Ableitung).

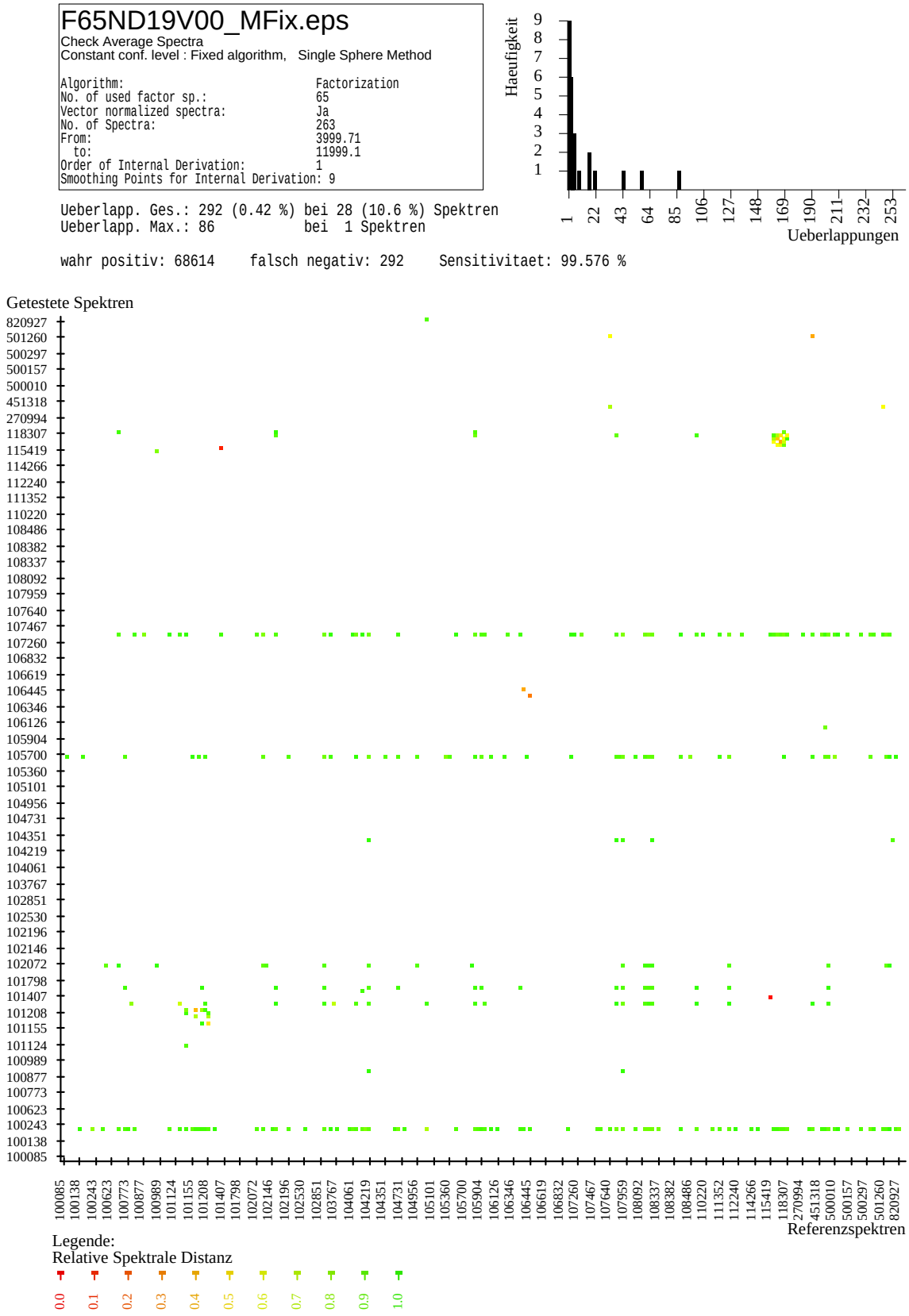


Abb. N11: Faktormethode (65 Faktoren, Vektornormierung und 1. Ableitung).

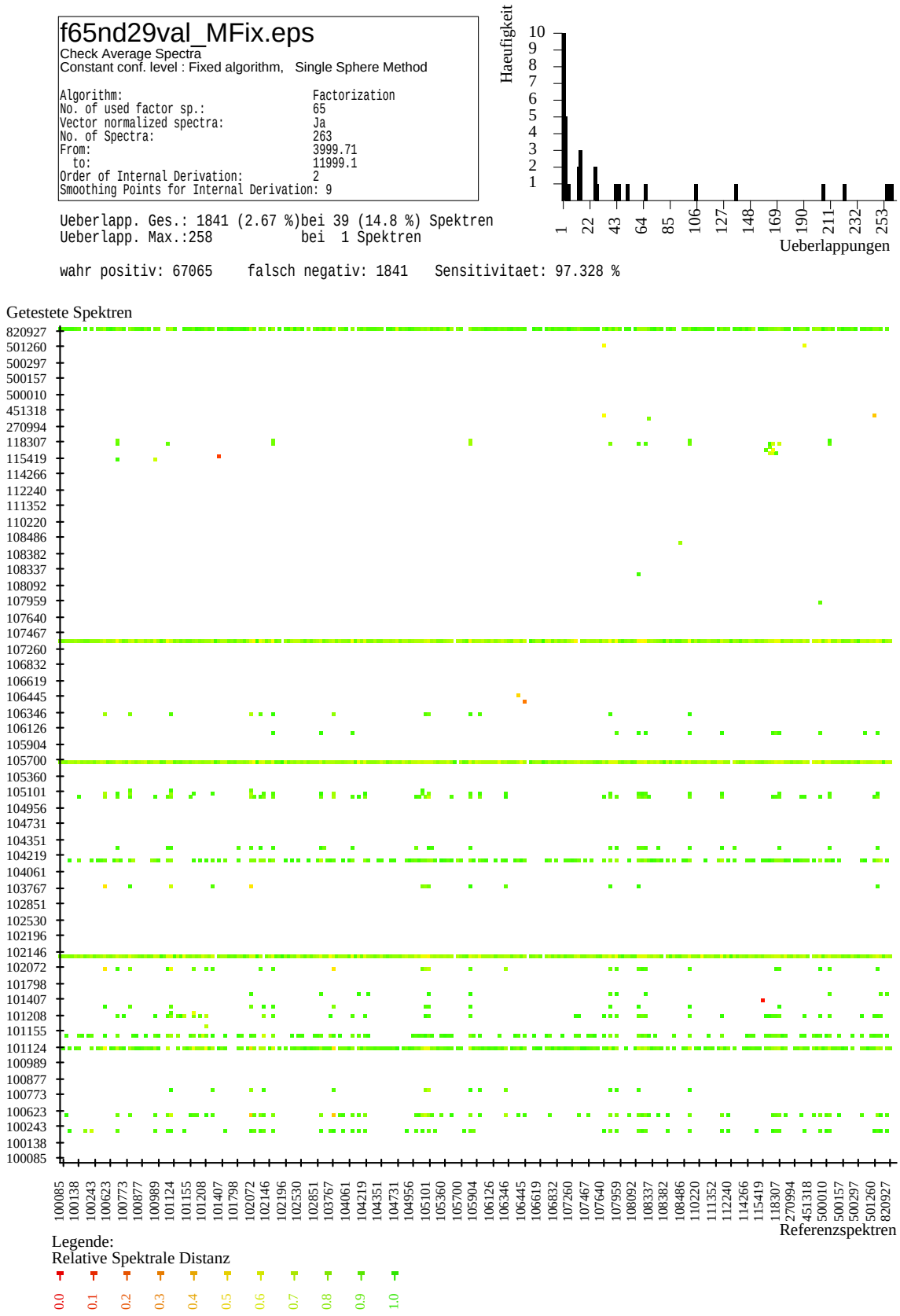


Abb. N12: Faktormethode (65 Faktoren, Vektornormierung und 2. Ableitung).

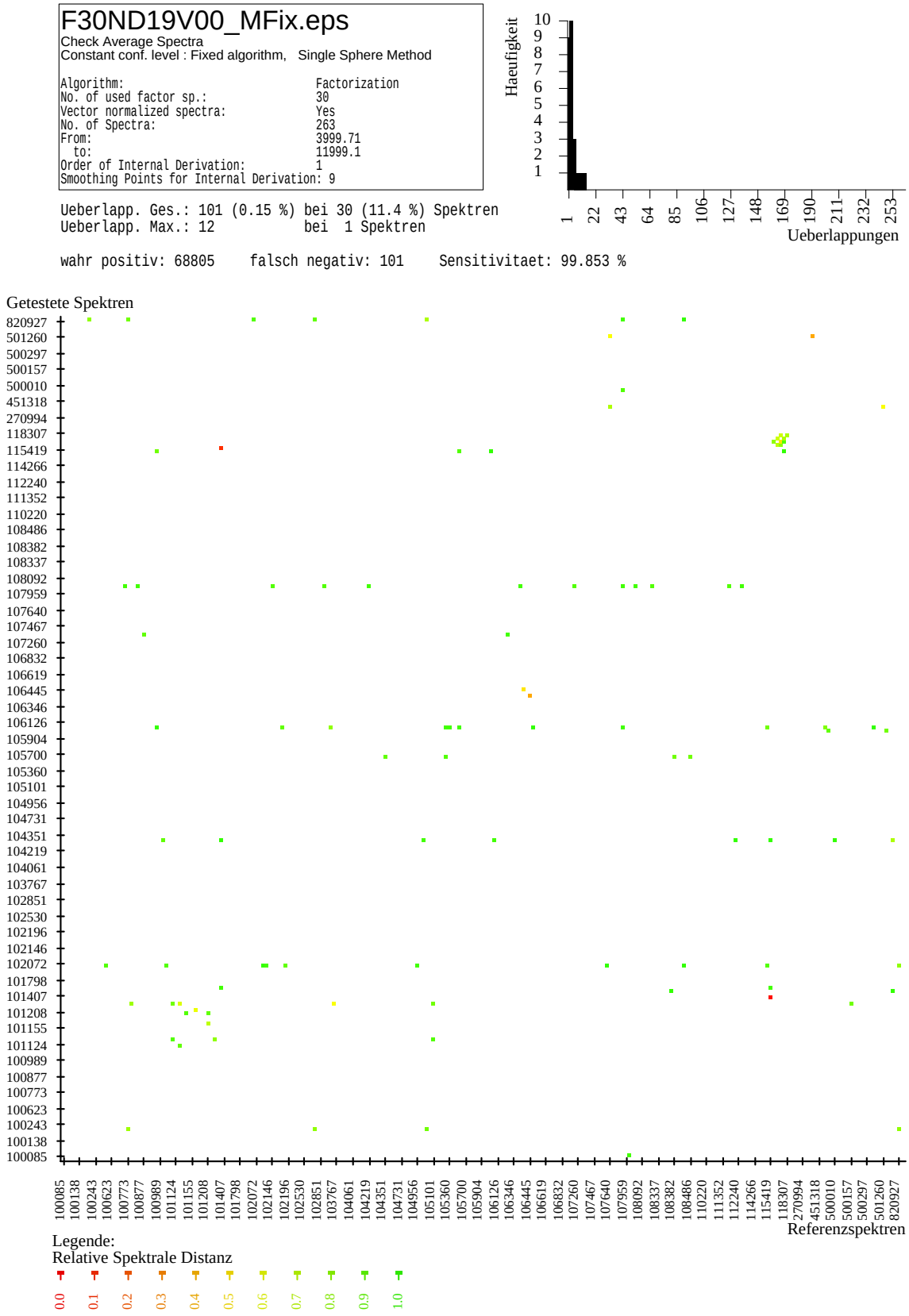


Abb. N13: Faktormethode (30 Faktoren, Vektornormierung und 1. Ableitung).

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

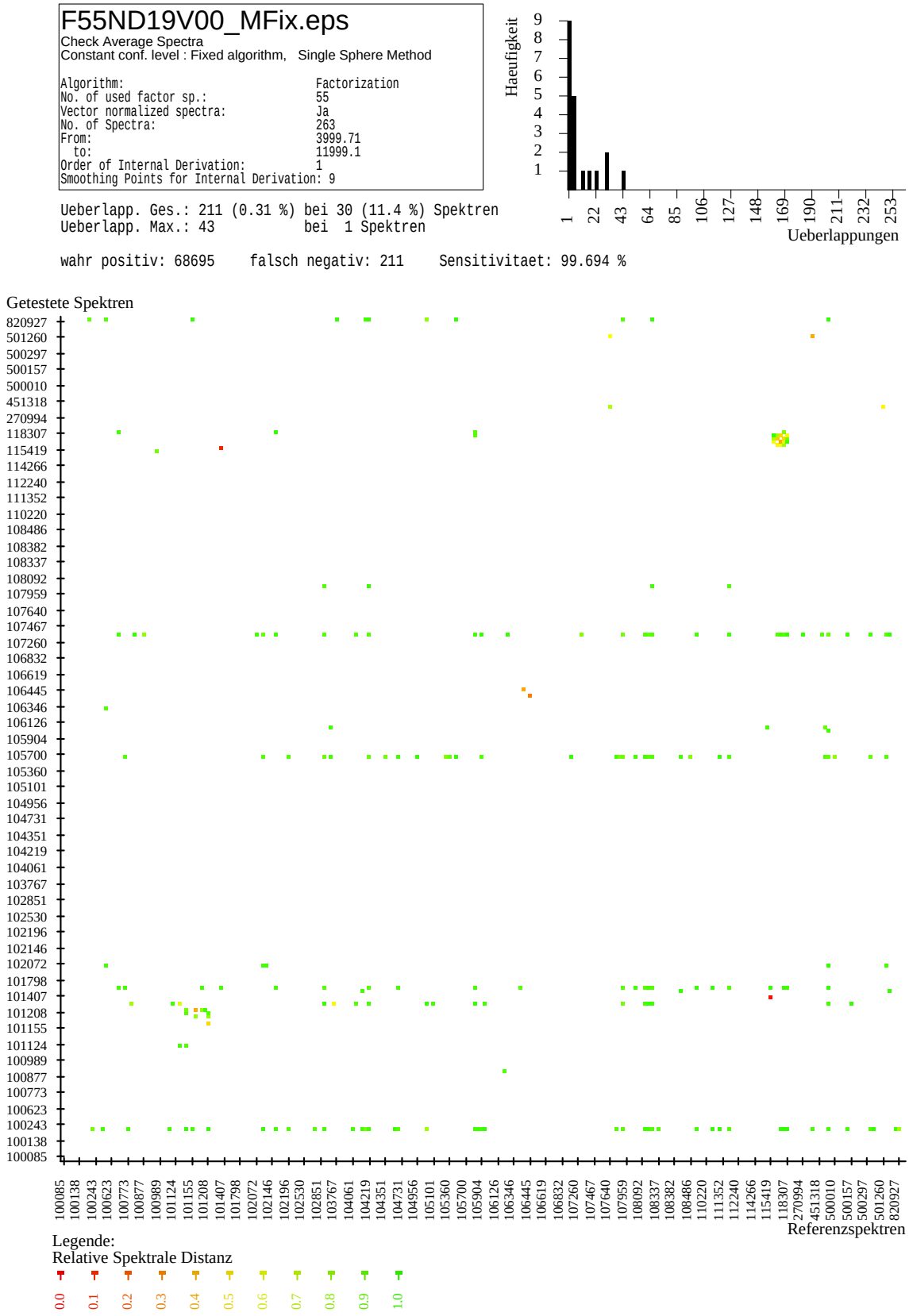


Abb. N15: Faktormethode (55 Faktoren, Vektornormierung und 1. Ableitung).

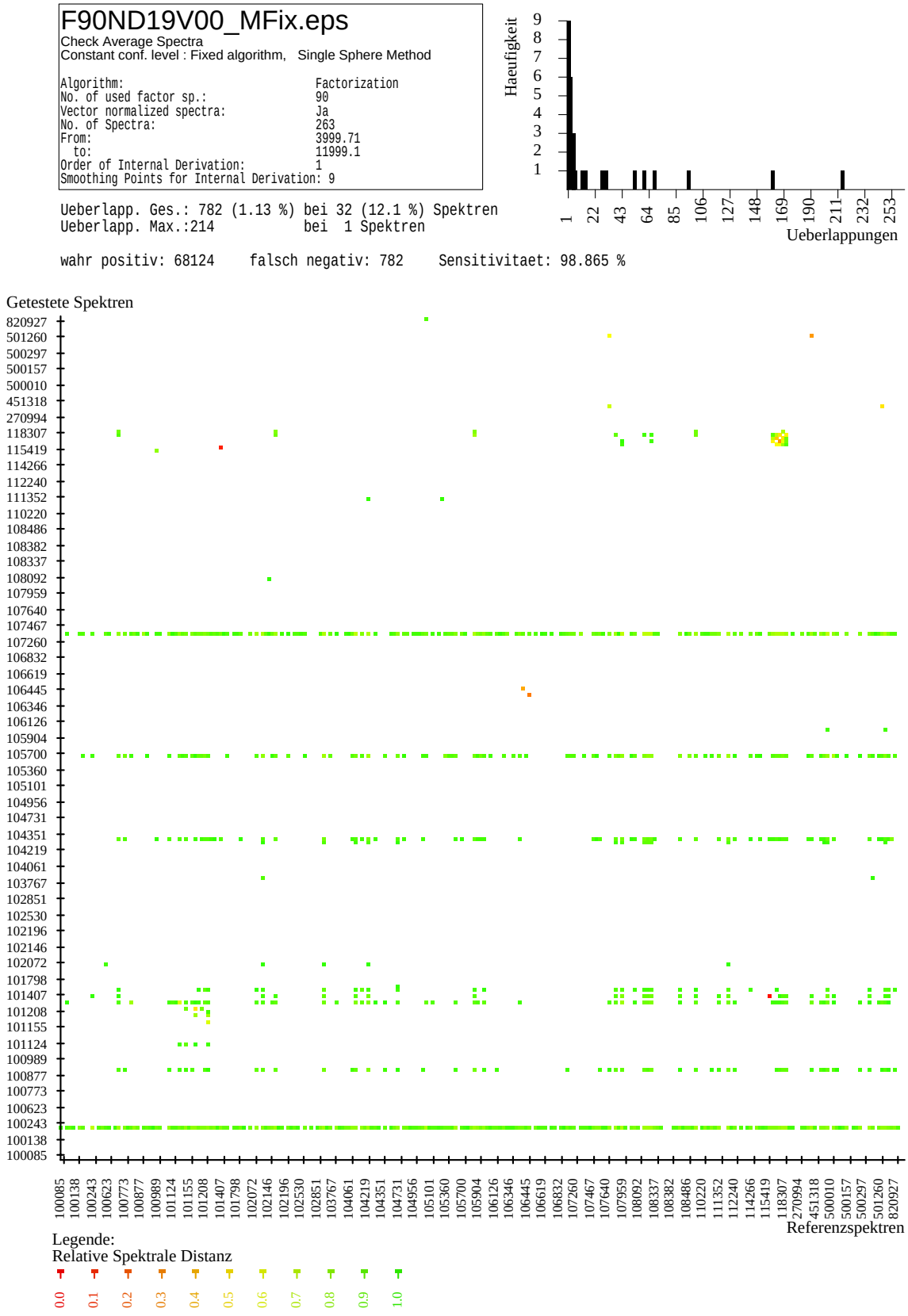


Abb. N16: Faktormethode (90 Faktoren, Vektornormierung und 1. Ableitung).

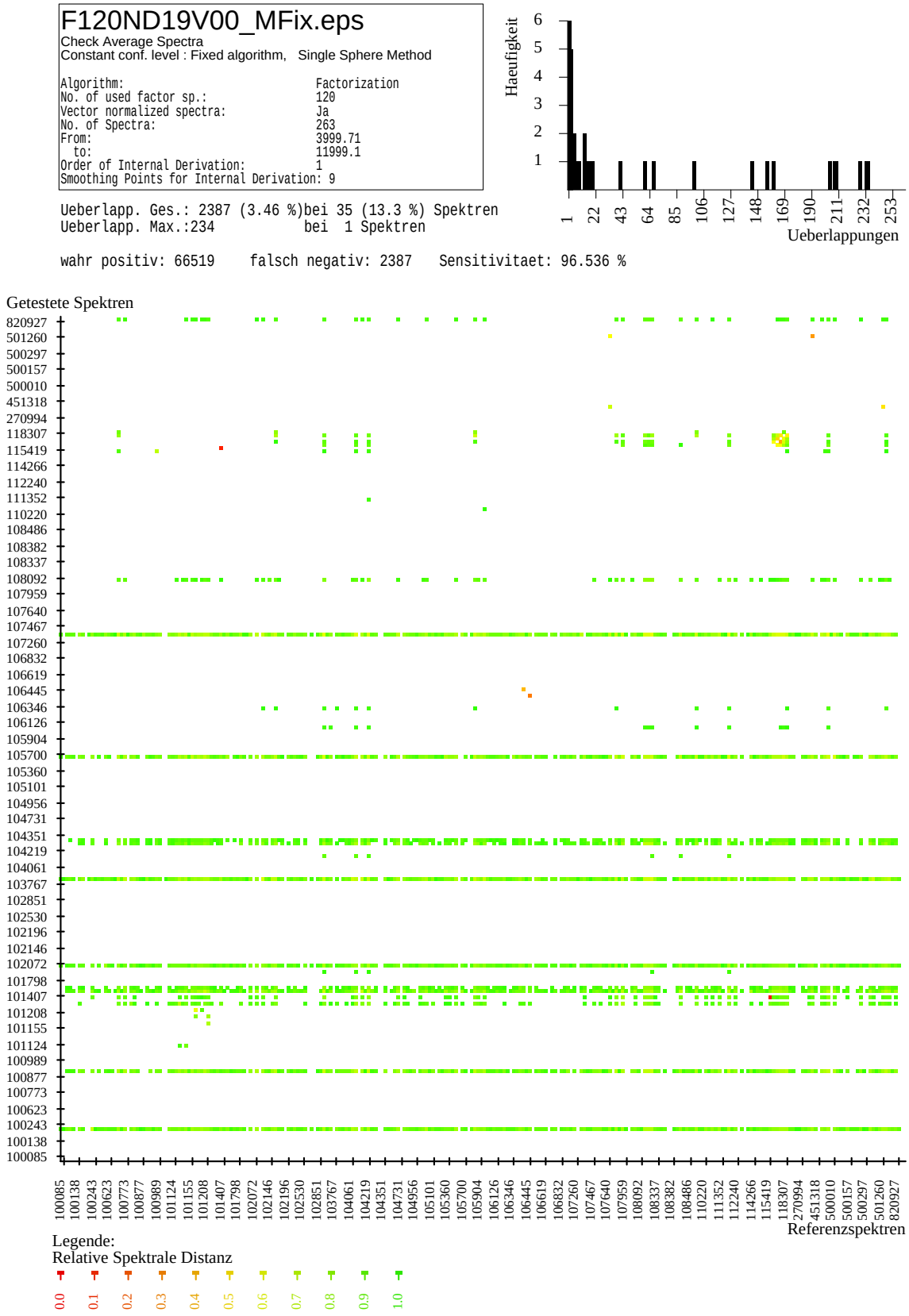


Abb. N17: Faktormethode (120 Faktoren, Vektornormierung und 1. Ableitung).

7.4.3 NIR, Variation des Spektralbereiches

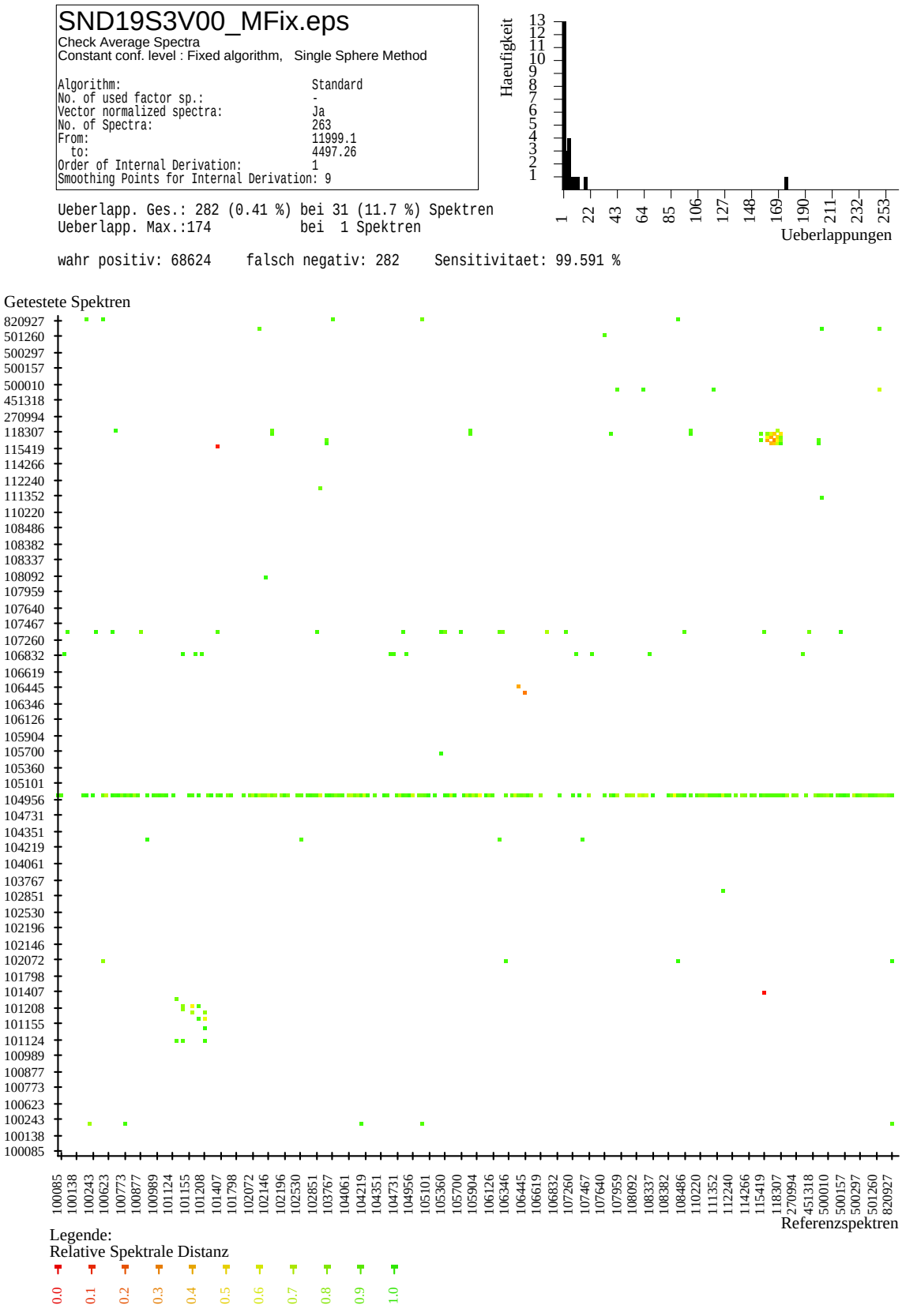


Abb. N18: Standardmethode (Vektornormierung und 1. Ableitung, 12000 cm^{-1} bis 4500 cm^{-1}).

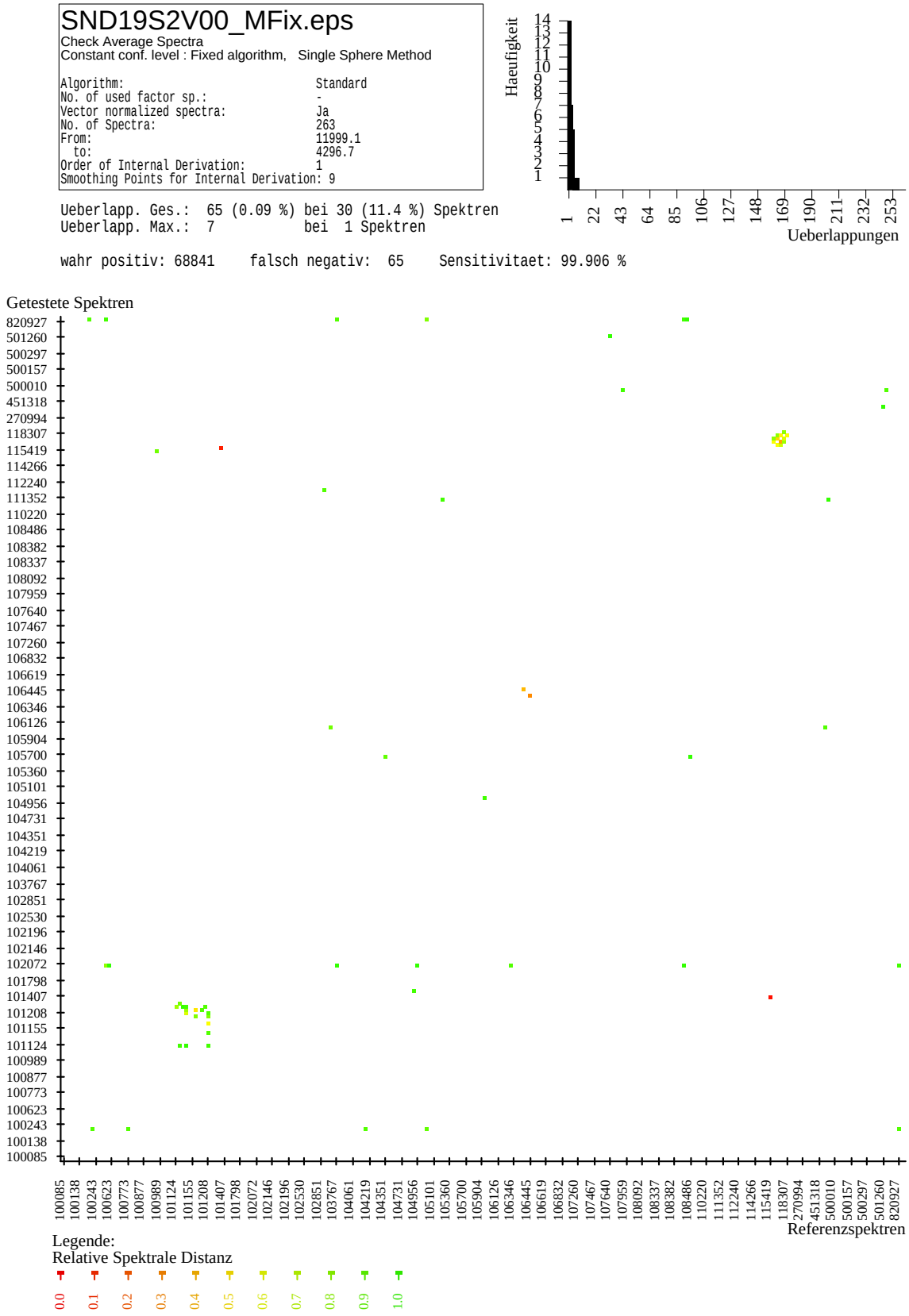


Abb. N19: Standardmethode (Vektornormierung und 1. Ableitung, 12000 cm-1 bis 4300 cm-1).

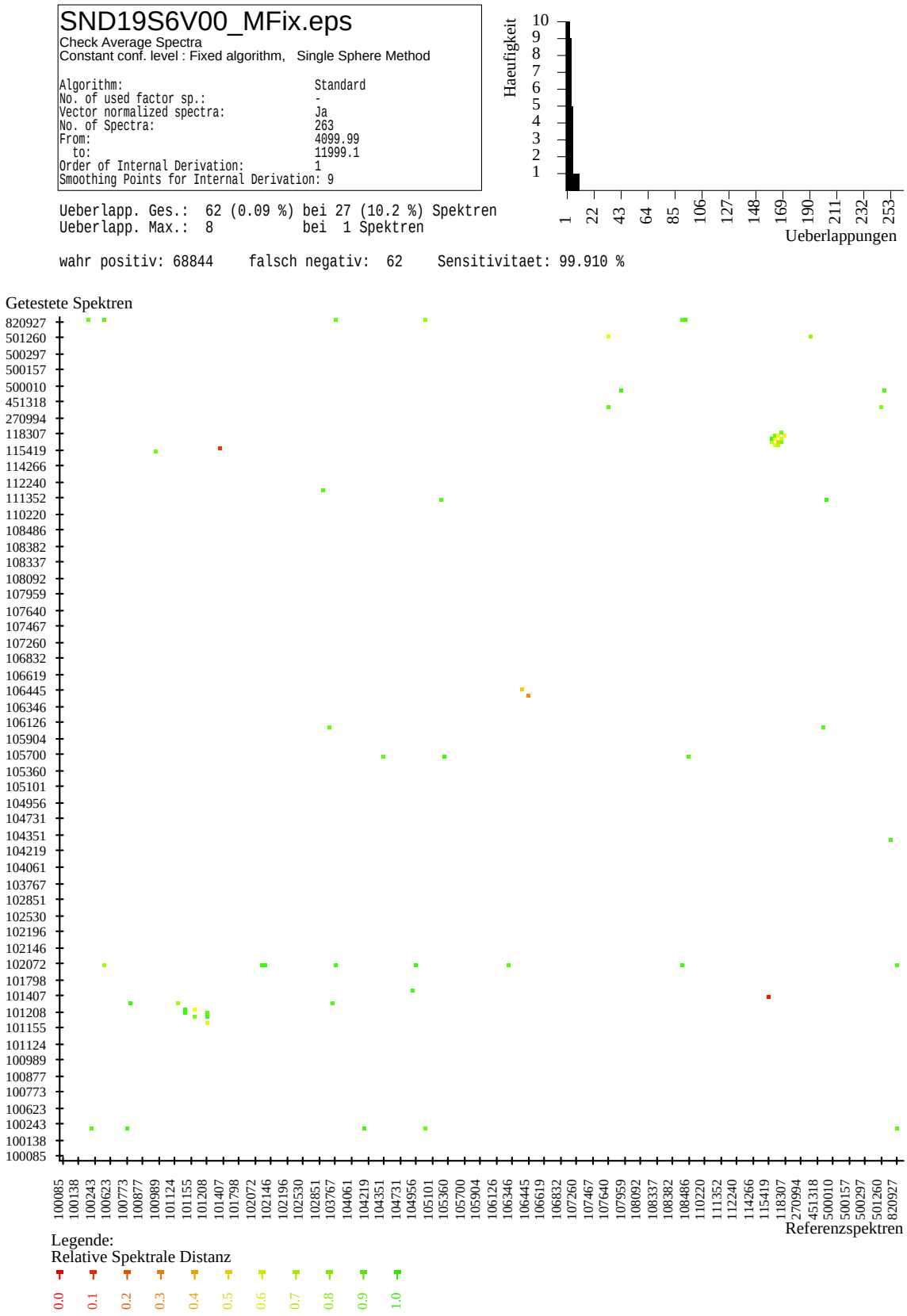


Abb. N20: Standardmethode (Vektornormierung und 1. Ableitung, 12000 cm^{-1} bis 4100 cm^{-1}).

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}).

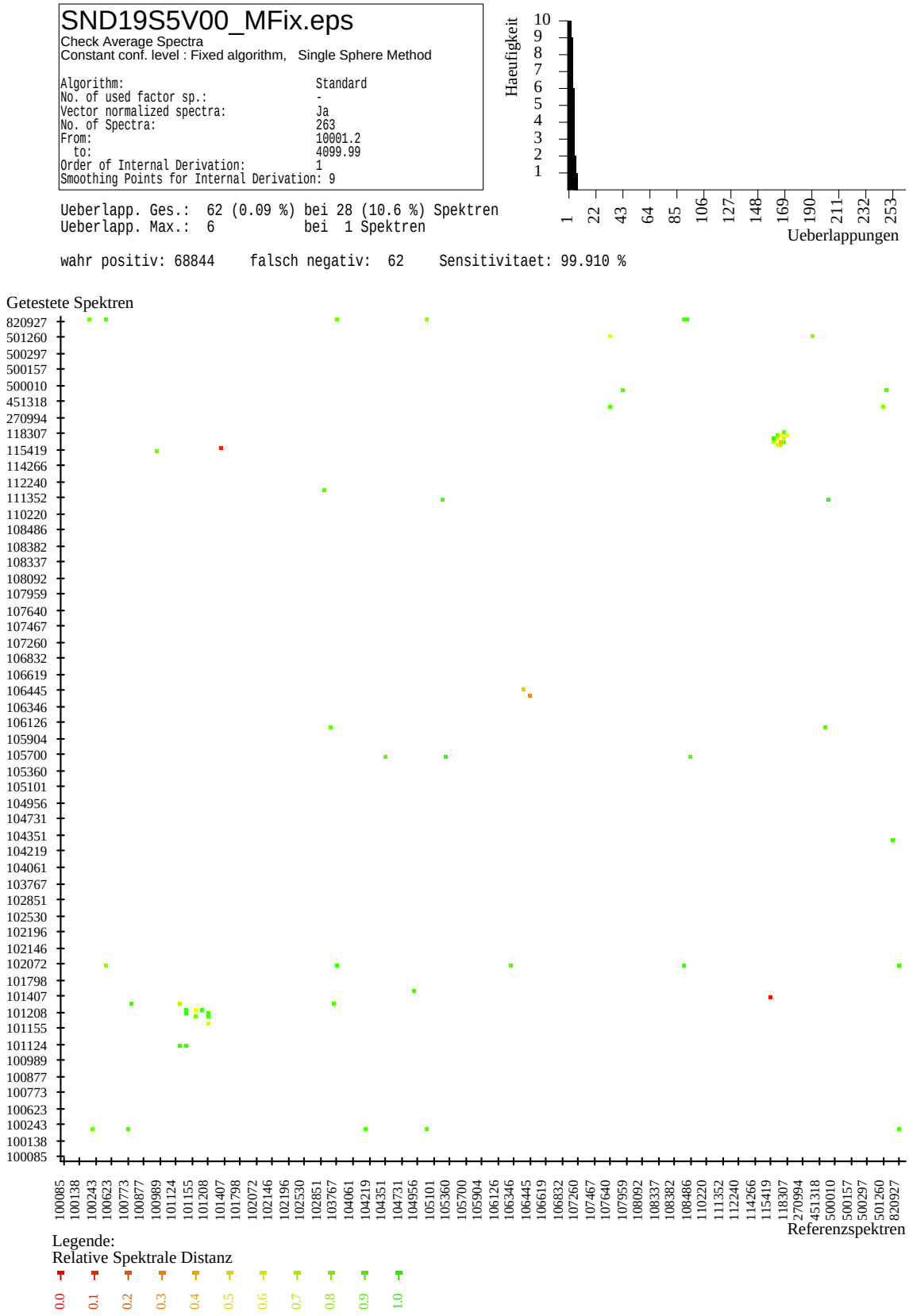


Abb. N23: Standardmethode (Vektornormierung und 1. Ableitung, 10000 cm^{-1} bis 4100 cm^{-1}).

7.4.4 NIR, Variation der Thresholdberechnung

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

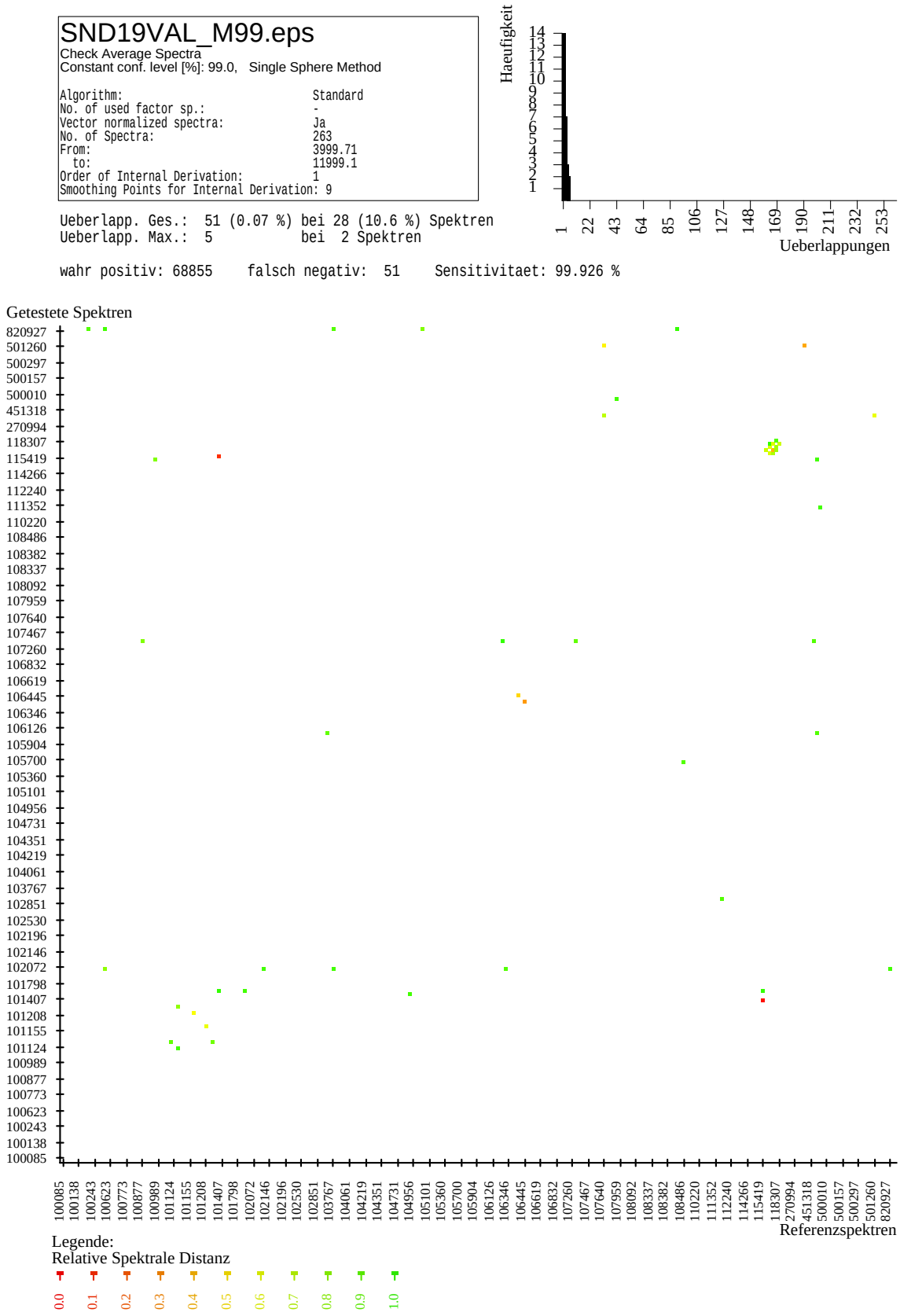


Abb. N25: Standardmethode (Vektornormierung und 1. Ableitung, konstantes Konfidenzniveau von 99 %).

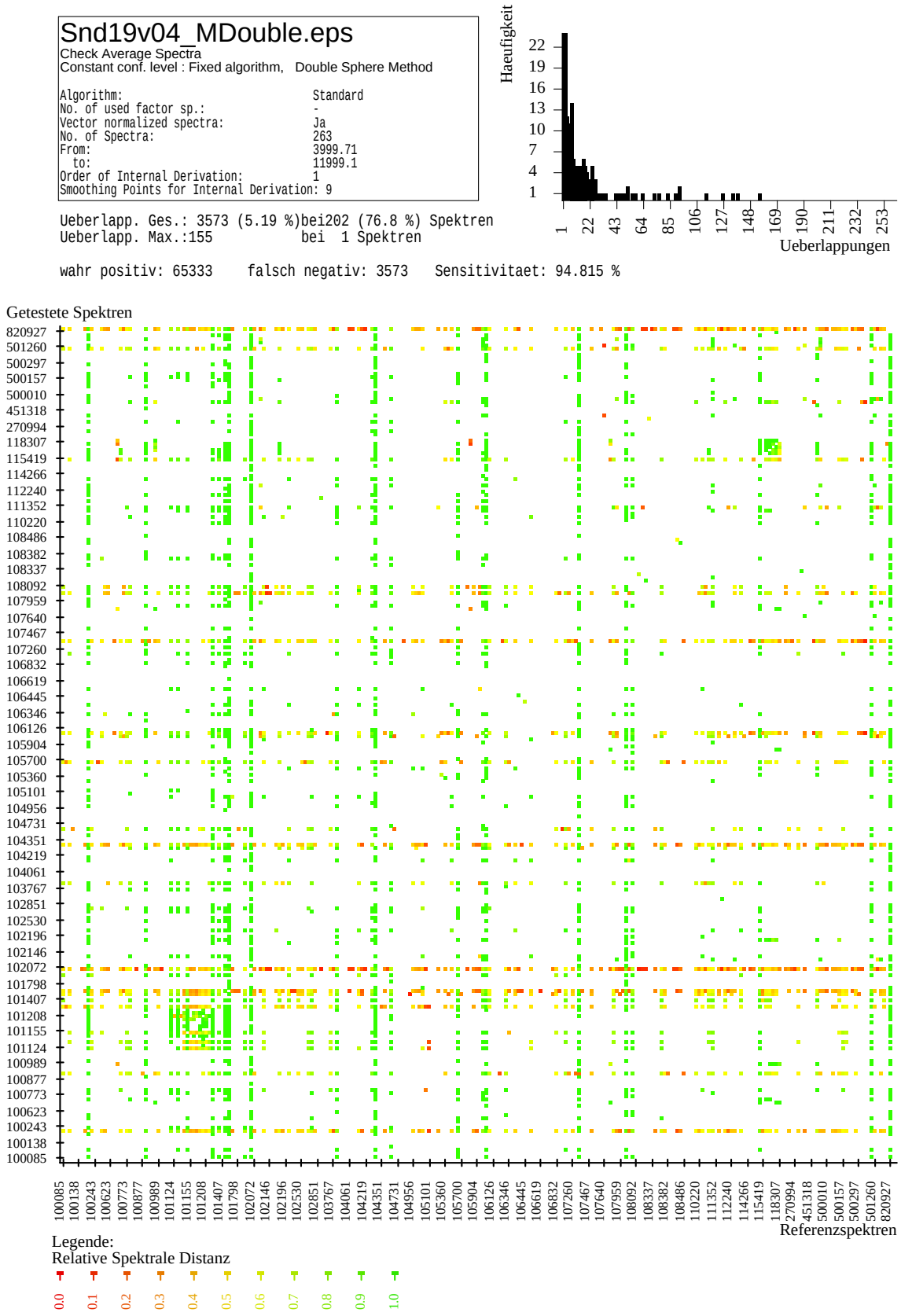


Abb. N26: Standardmethode (Vektornormierung und 1. Ableitung, Doppelkugelmodell, Fixed Algorithm).

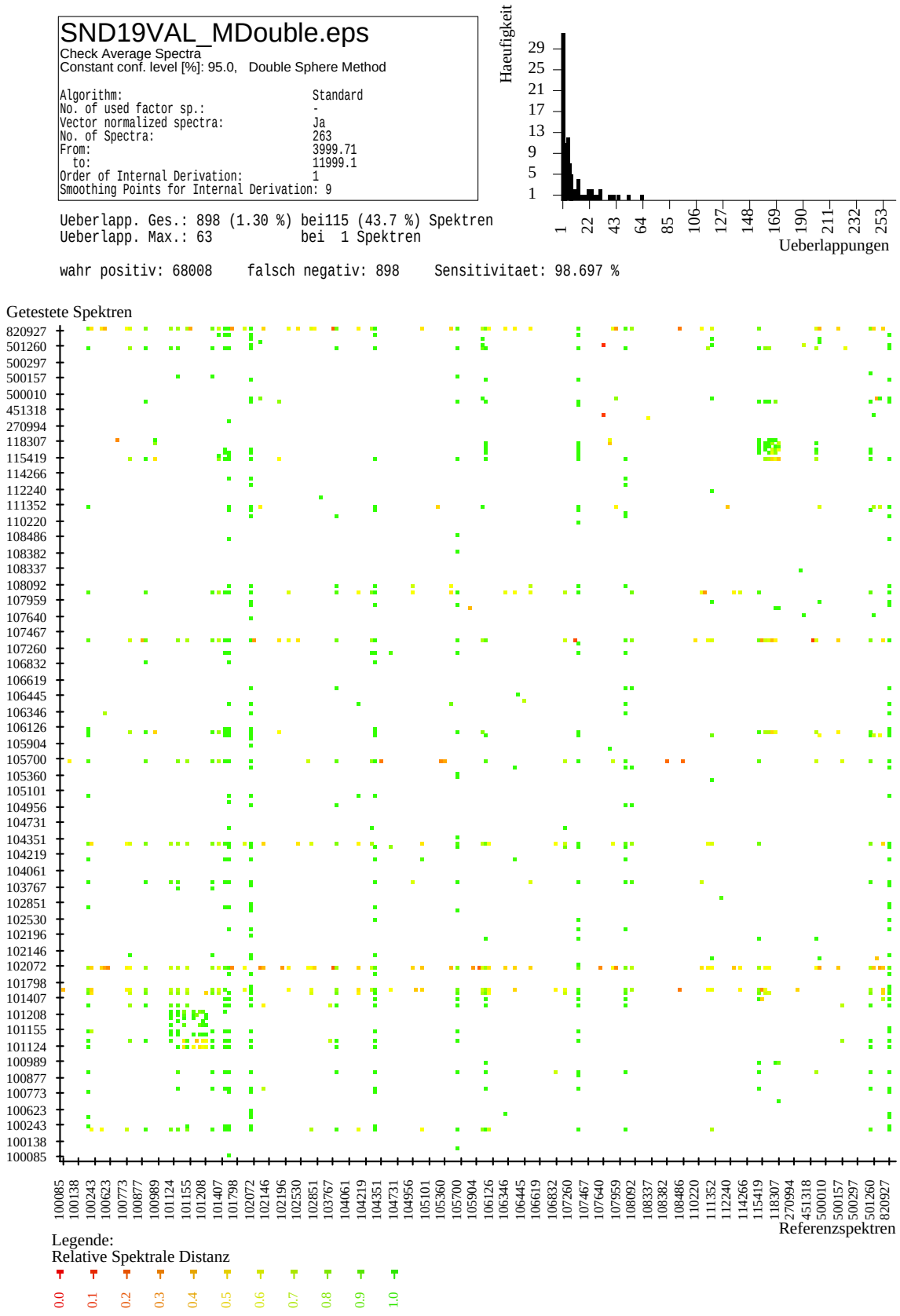


Abb. N27: Standardmethode (Vektornormierung und 1. Ableitung, Doppelkugelmodell, konstantes Konfidenzniveau von 95 %).

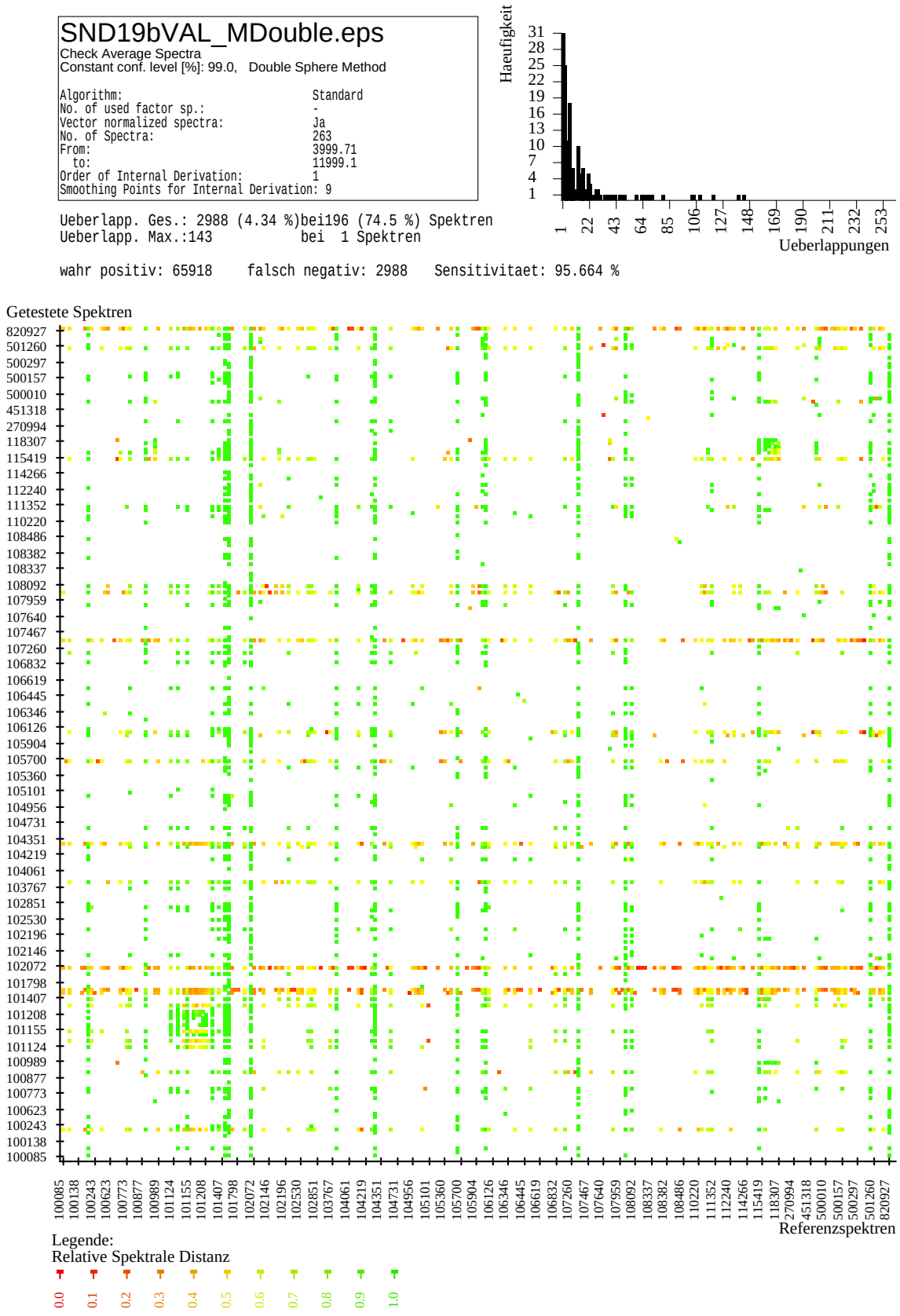


Abb. N28: Standardmethode (Vektornormierung und 1. Ableitung, Doppelkugelmodell, konstantes Konfidenzniveau von 99 %).

7.4.5 Raman, Standardmethode

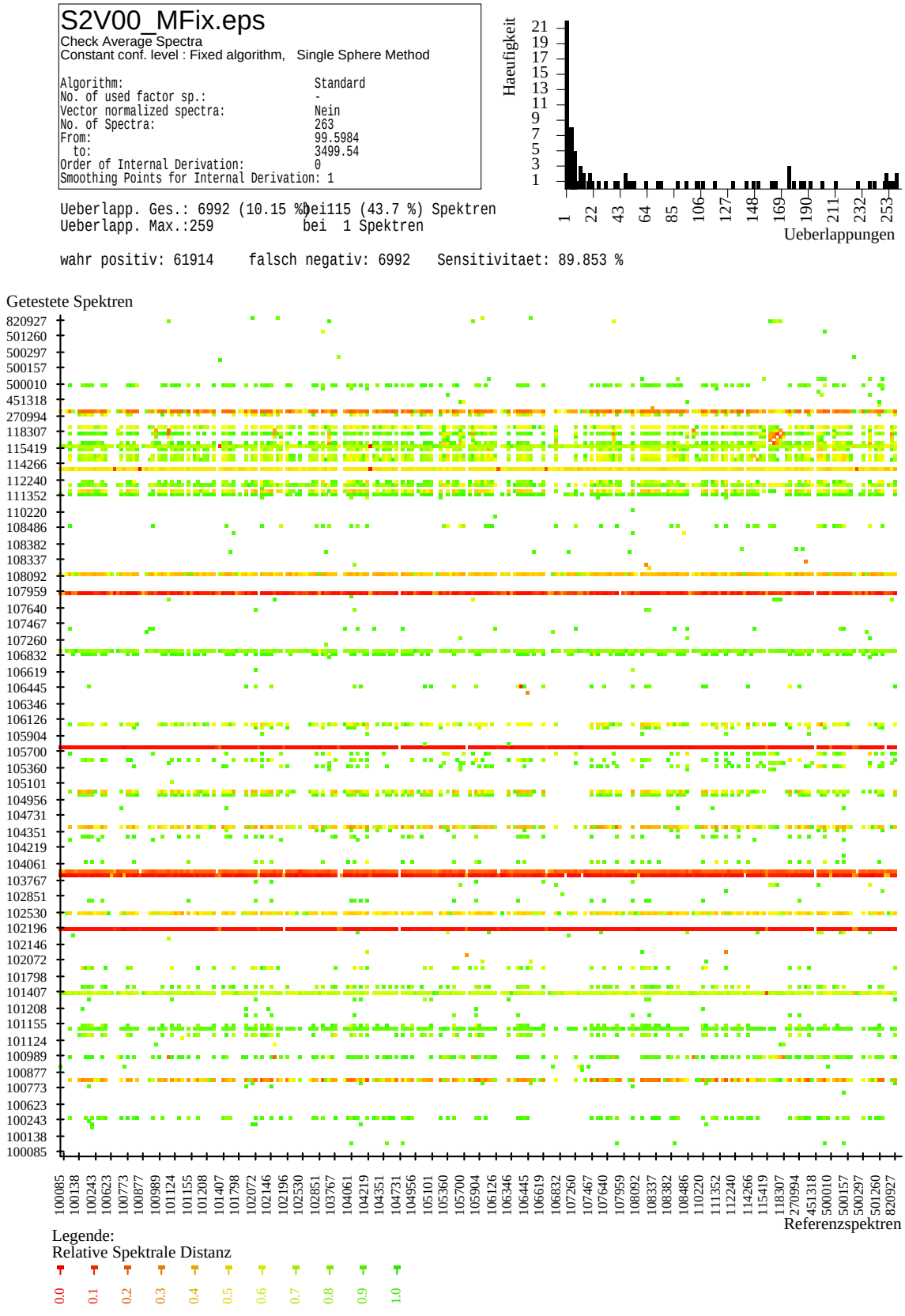


Abb. R1: Standardmethode.

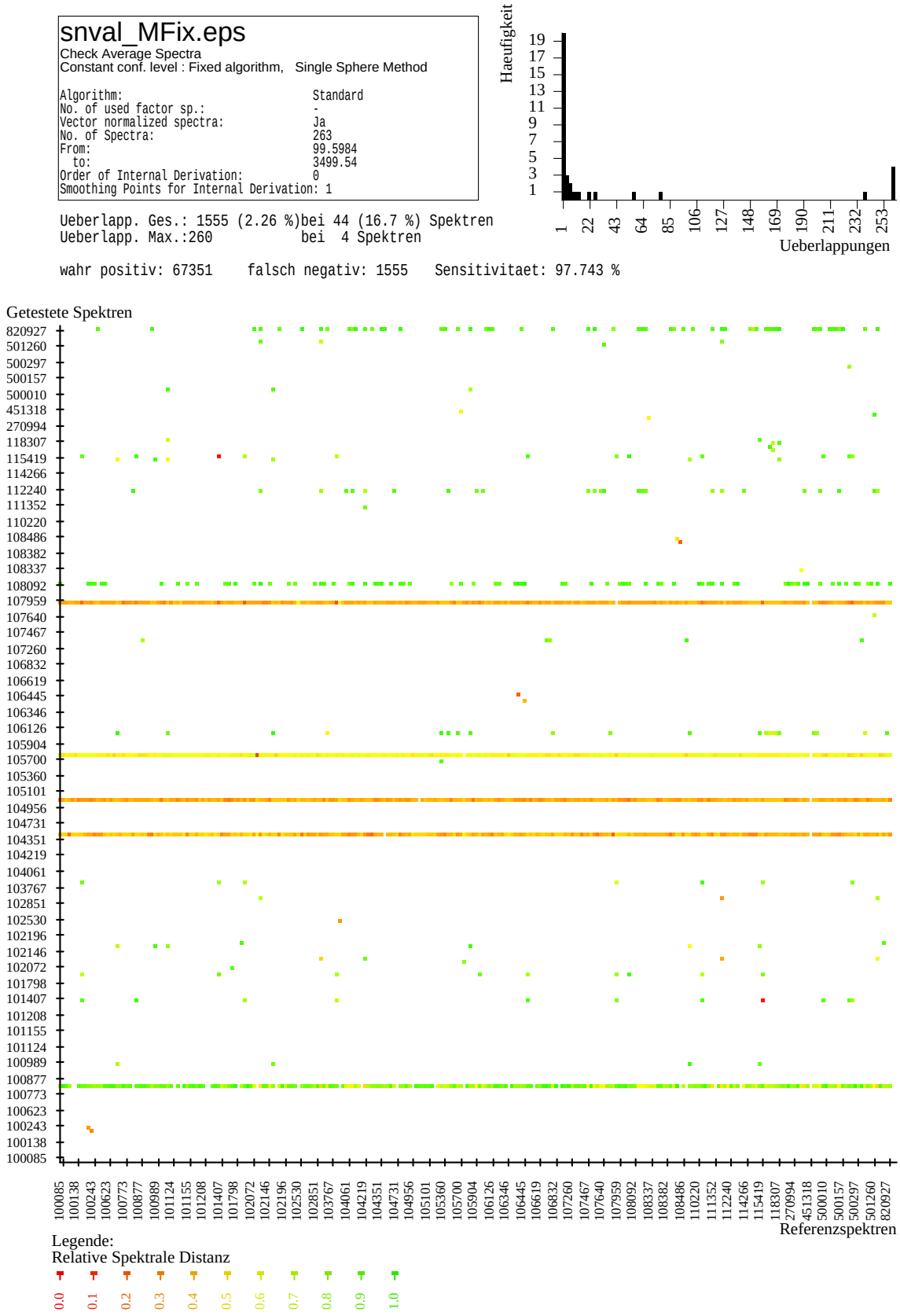


Abb. R2: Standardmethode (Vektornormierung).

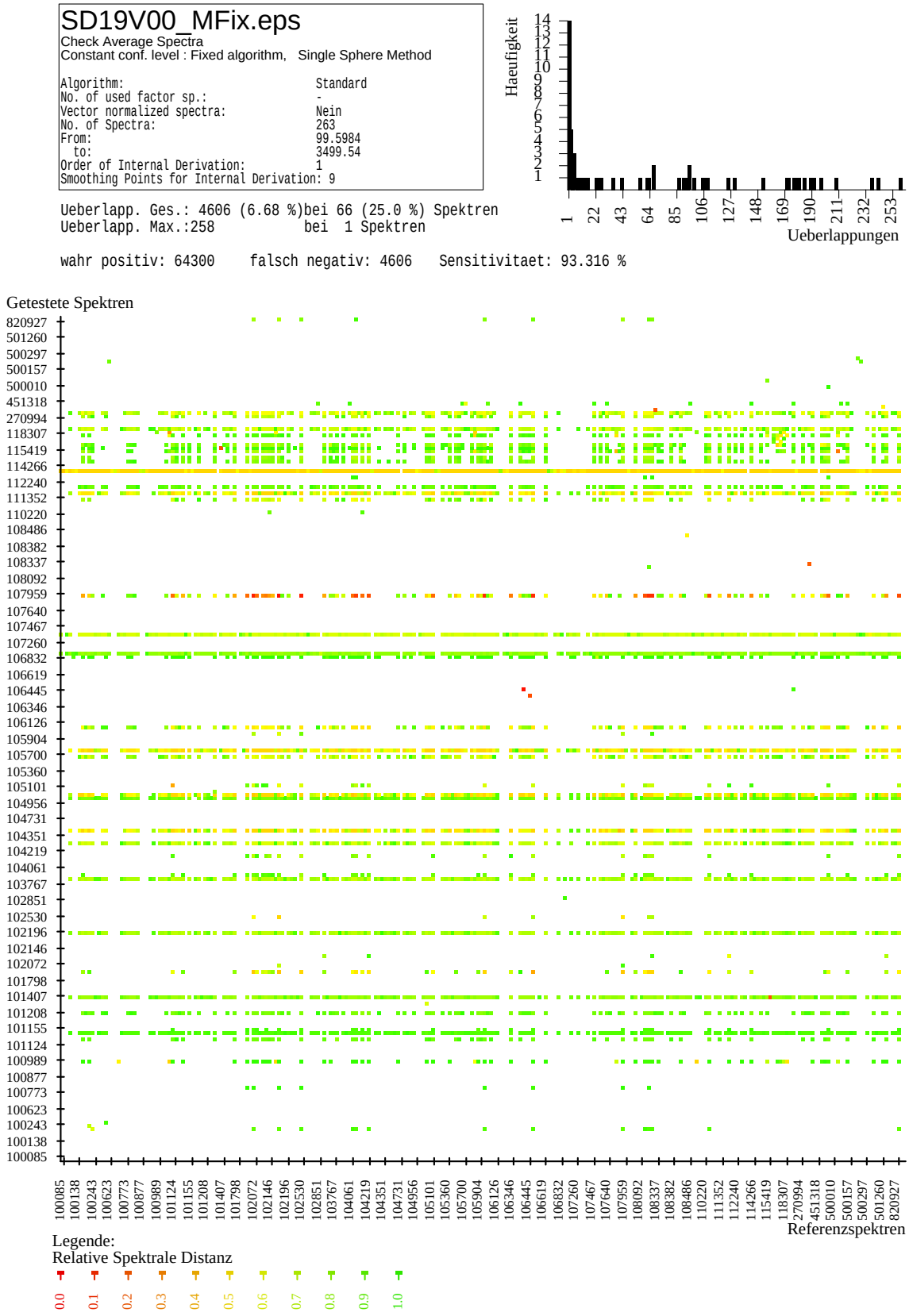


Abb. R3: Standardmethode (1. Ableitung).

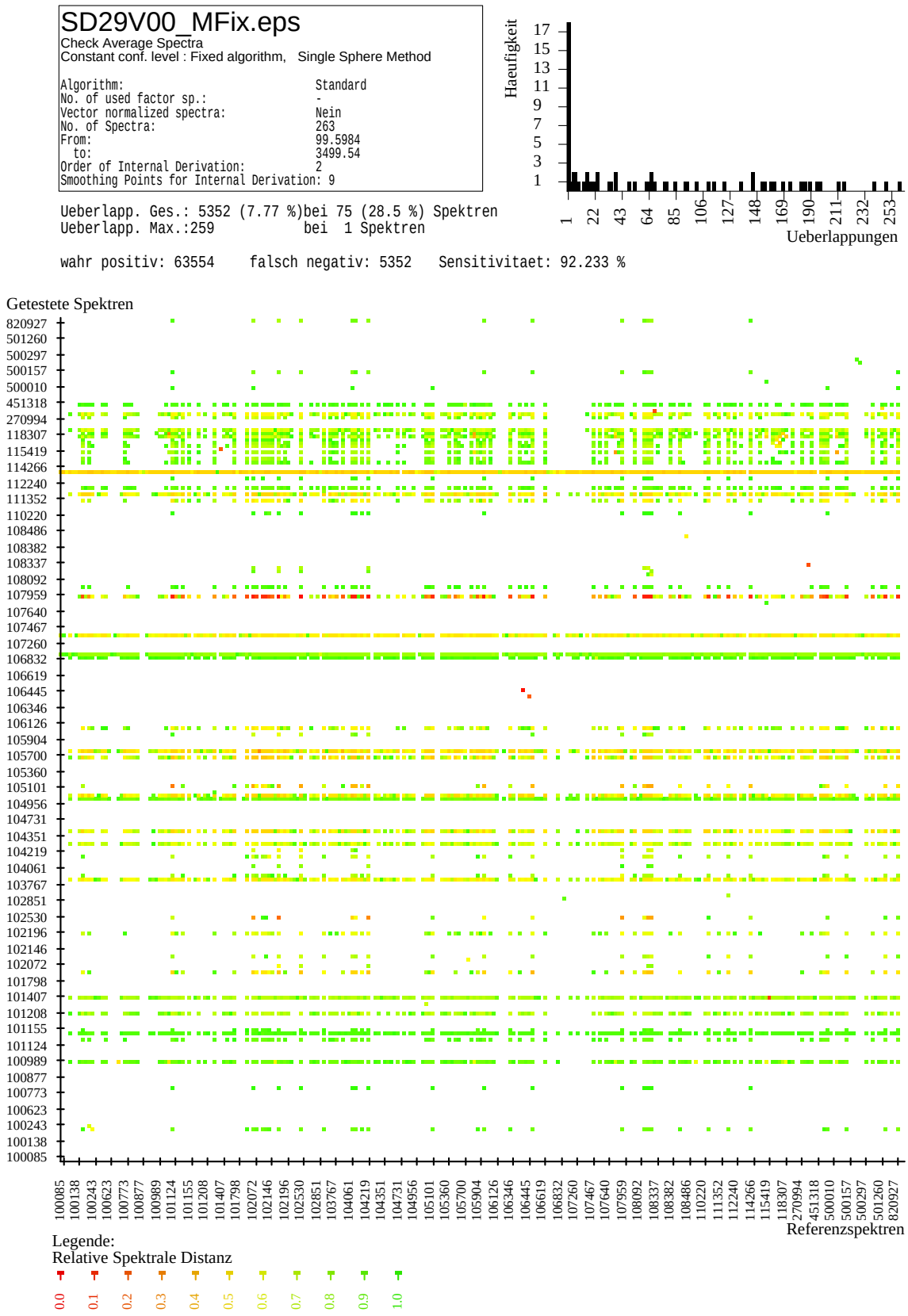


Abb. R4: Standardmethode (2. Ableitung).

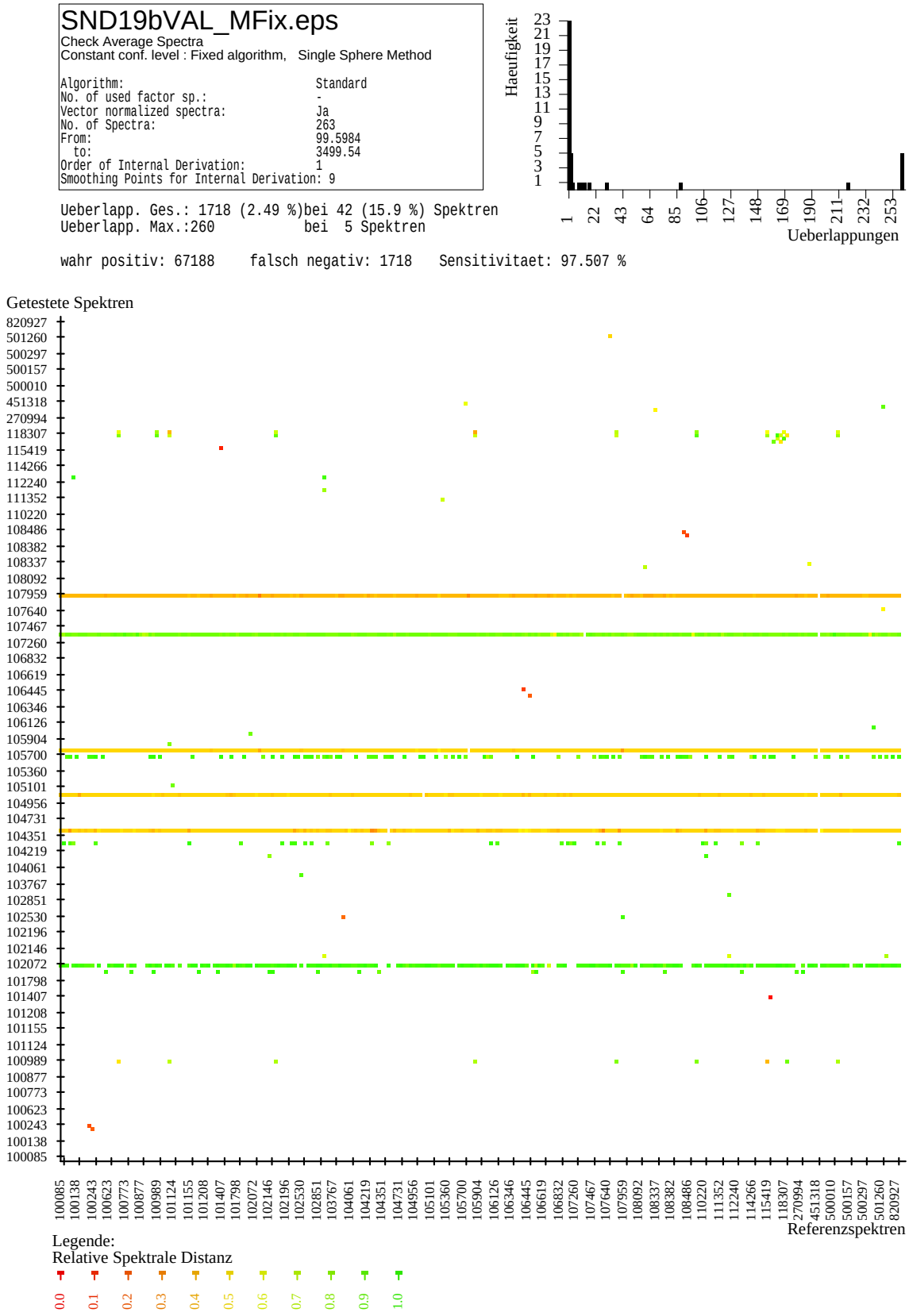


Abb. R5: Standardmethode (Vektornormierung und 1. Ableitung).

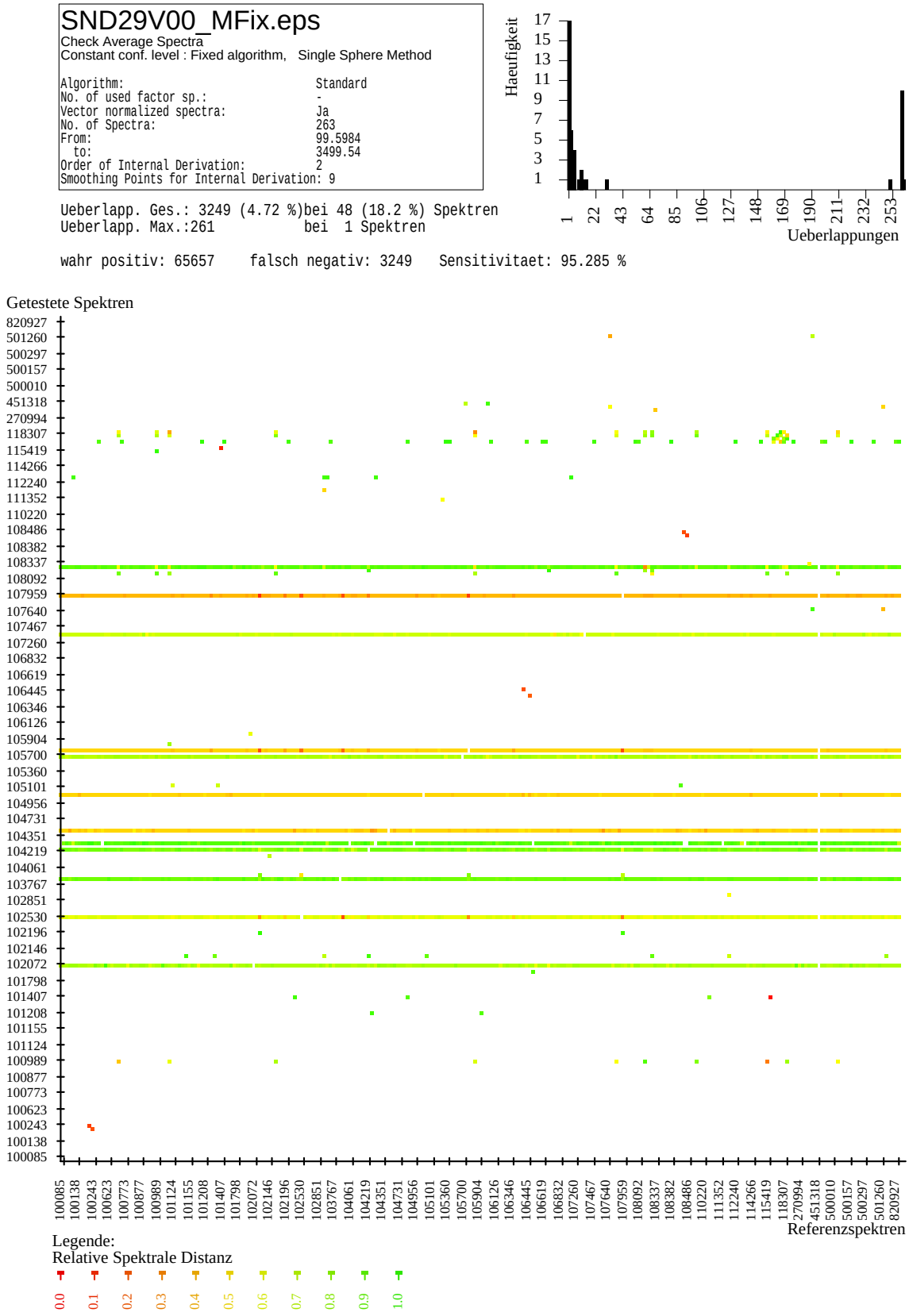


Abb. R6: Standardmethode (Vektornormierung und 2. Ableitung).

7.4.6 Raman, Faktormethode

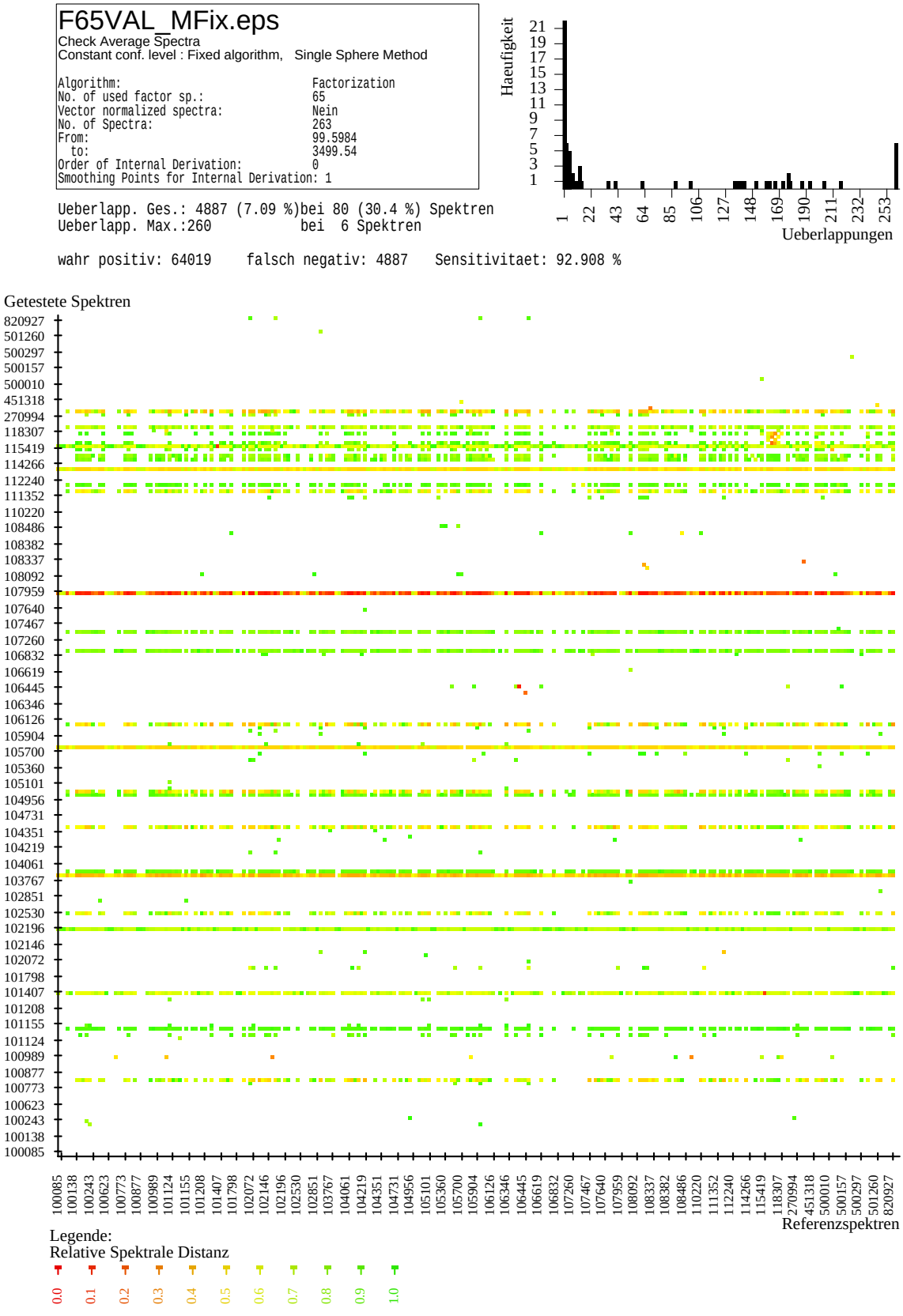


Abb. R7: Faktormethode (65 Faktoren).

Abb. R8: Faktormethode (65 Faktoren, Vektornormierung).

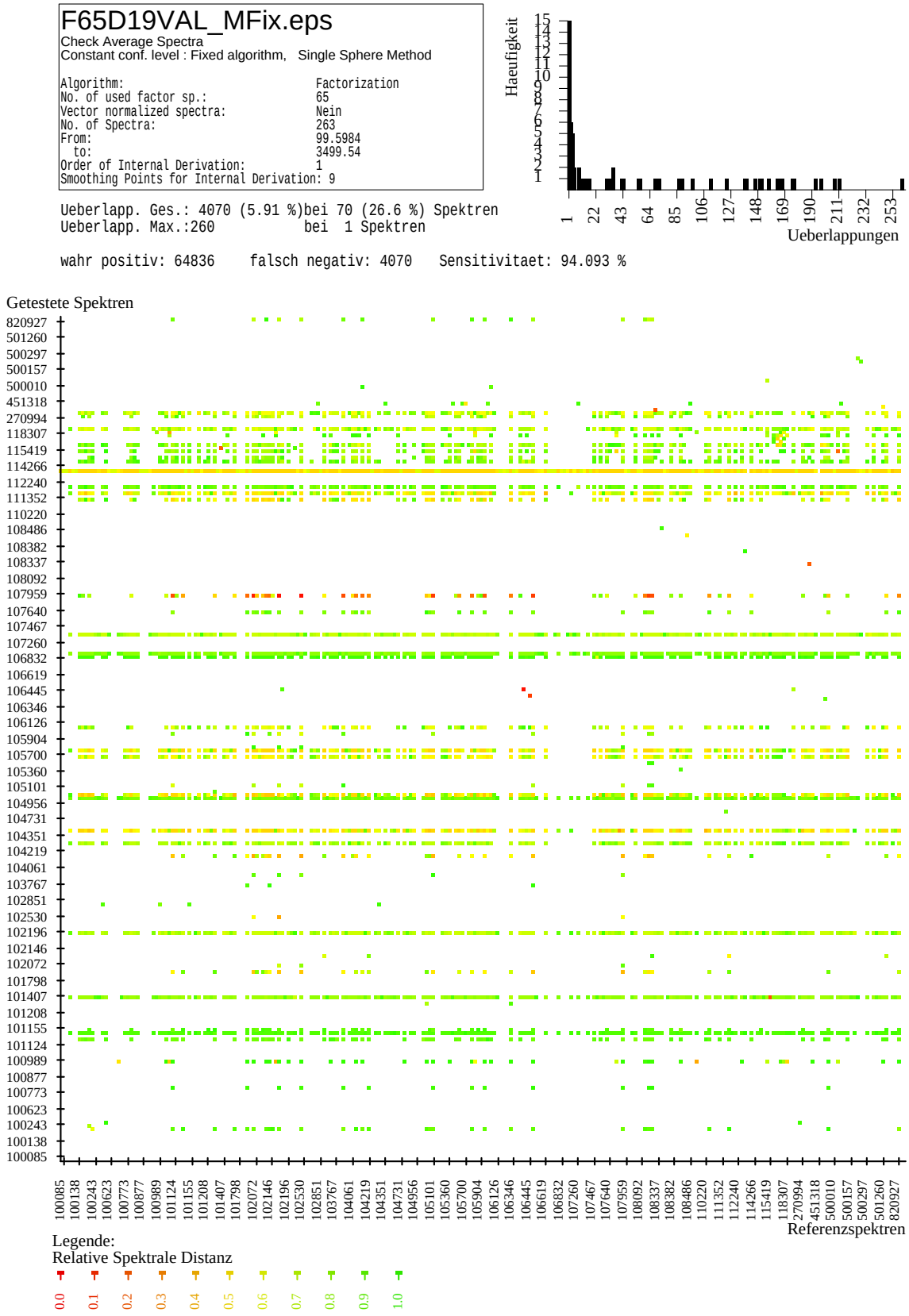


Abb. R9: Faktormethode (65 Faktoren, 1. Ableitung).

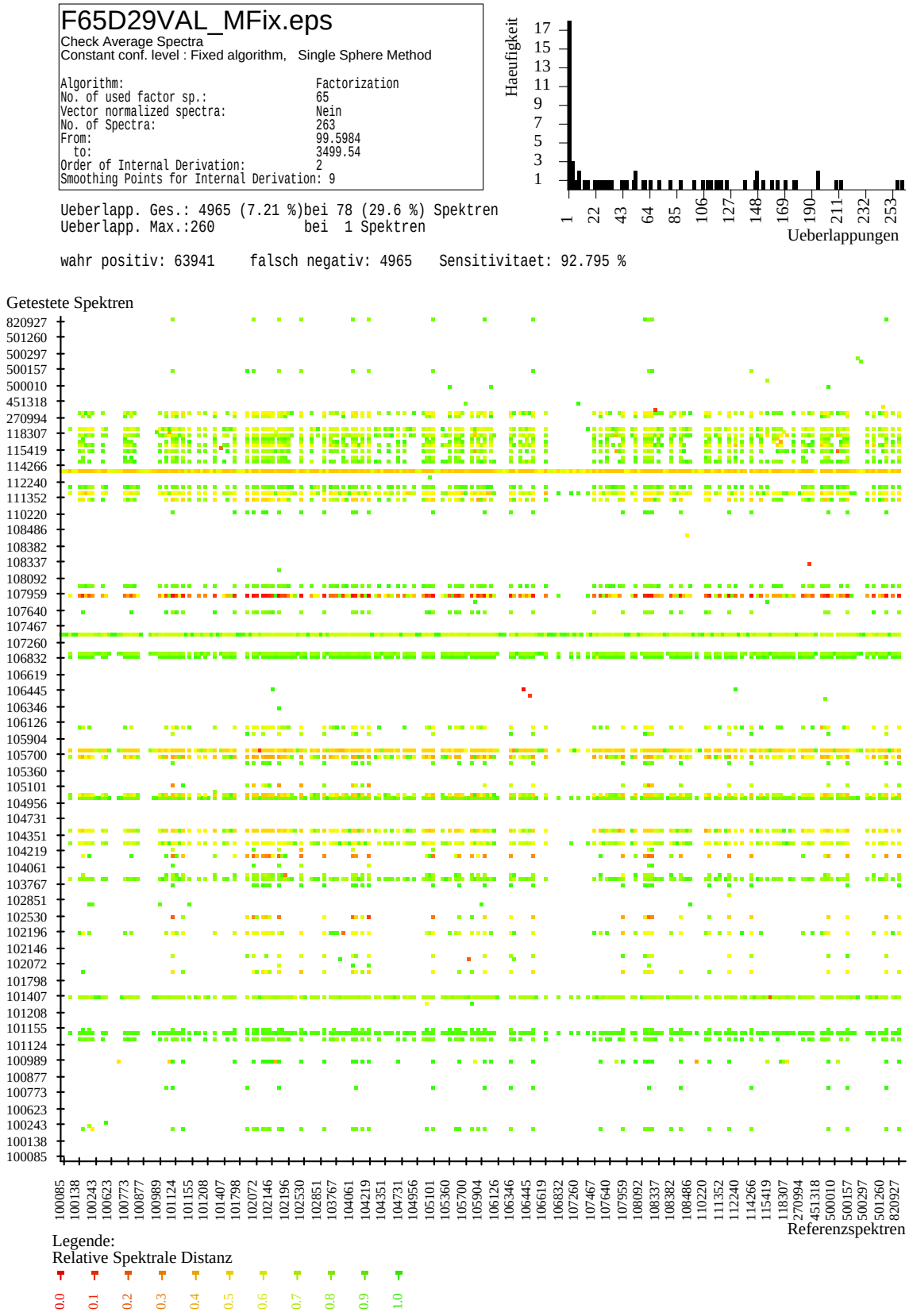


Abb. R10: Faktormethode (65 Faktoren, 2. Ableitung).

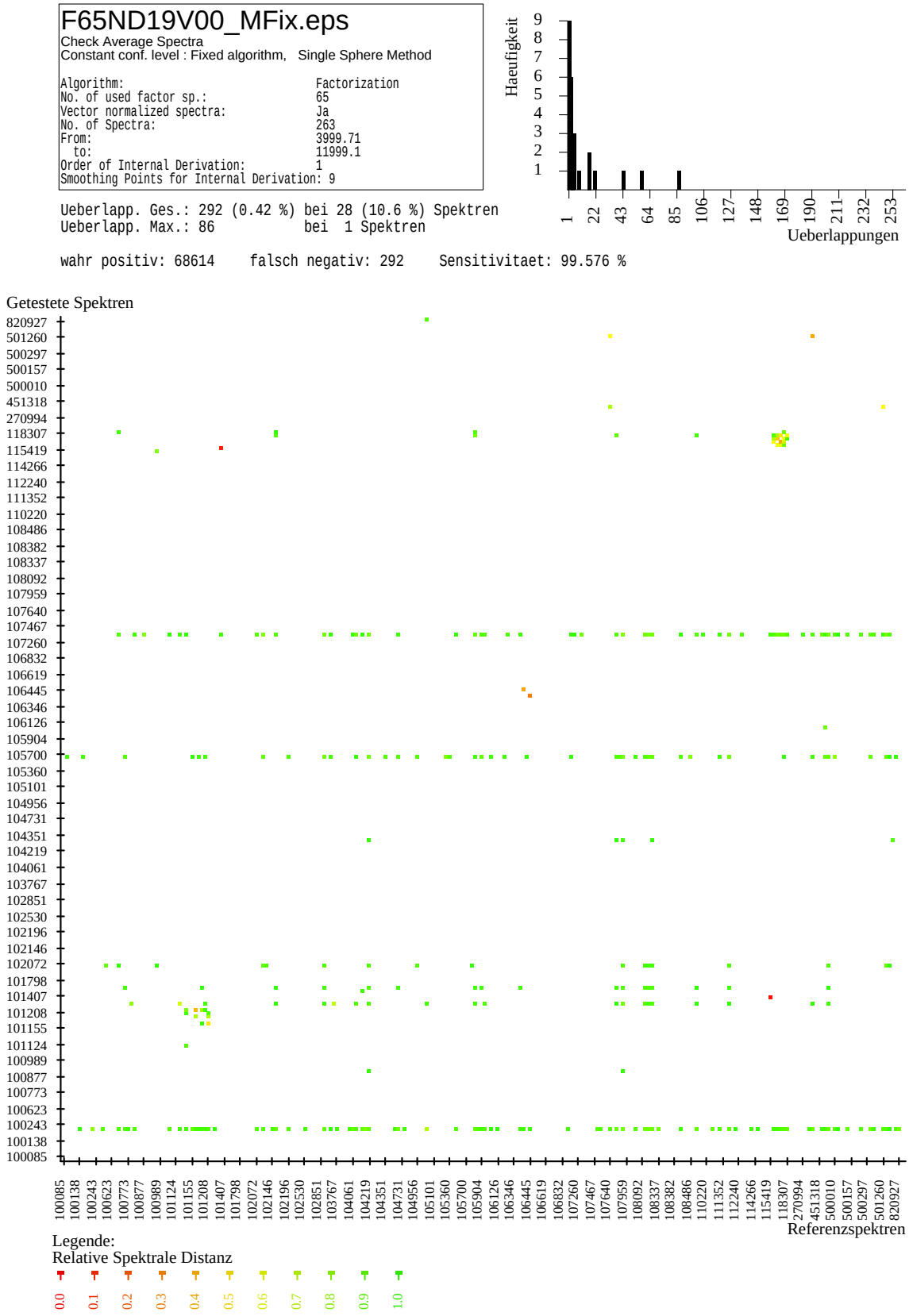


Abb. R11: Faktormethode (65 Faktoren, Vektornormierung, 1. Ableitung).

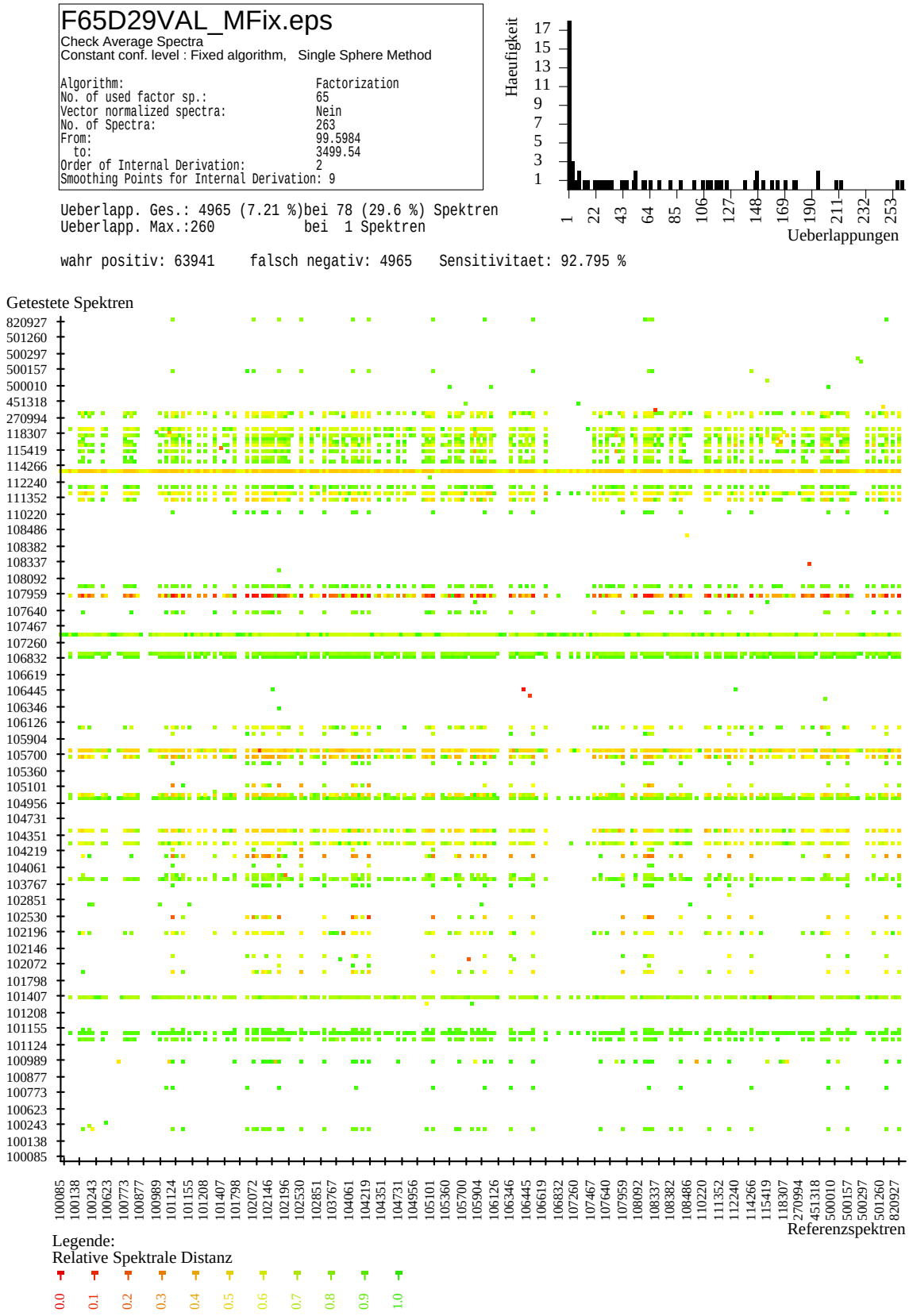


Abb. R12: Faktormethode (65 Faktoren, Vektornormierung, 2. Ableitung).

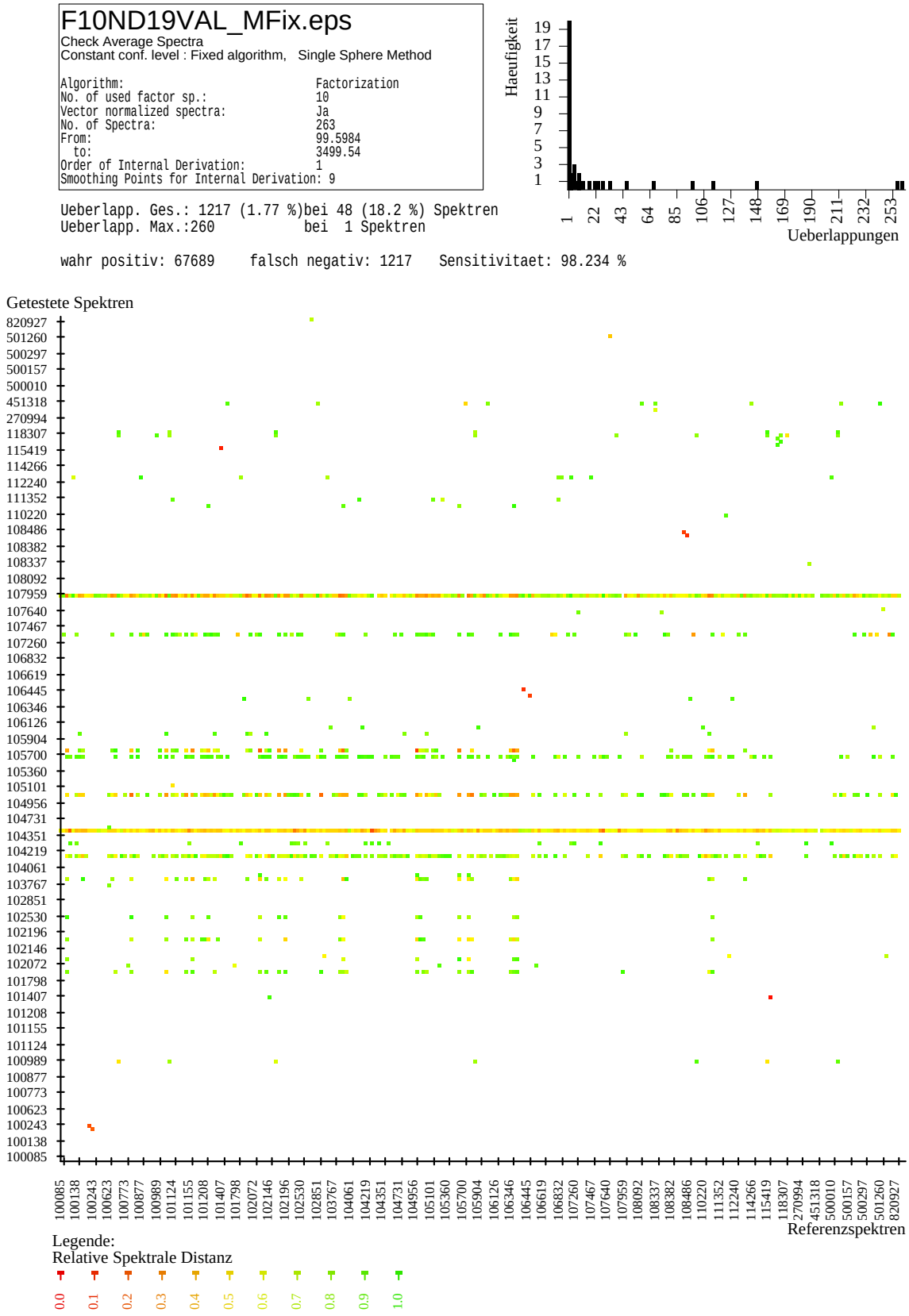


Abb. R13: Faktormethode (10 Faktoren, Vektornormierung, 1. Ableitung).

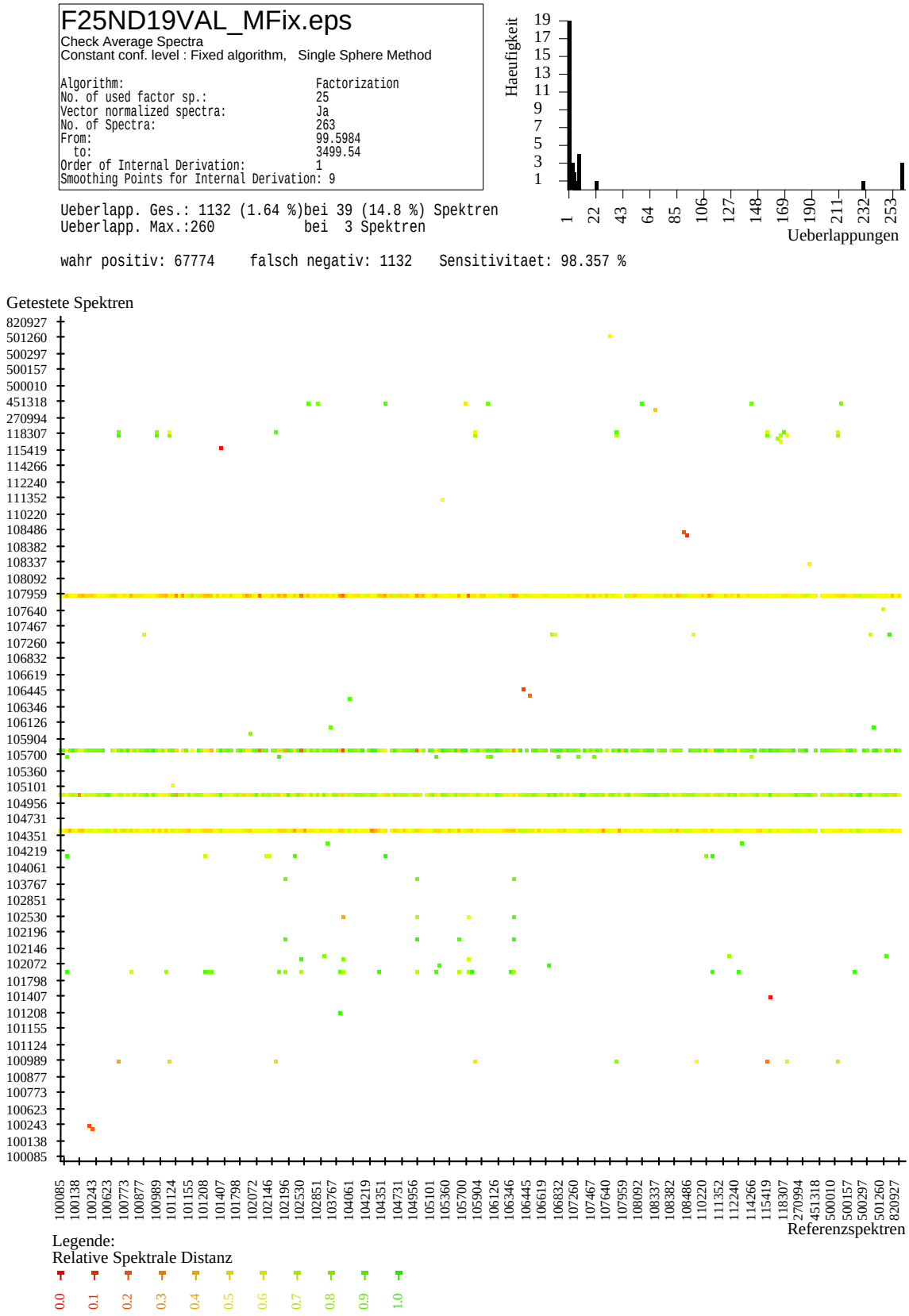


Abb. R14: Faktormethode (25 Faktoren, Vektornormierung, 1. Ableitung).

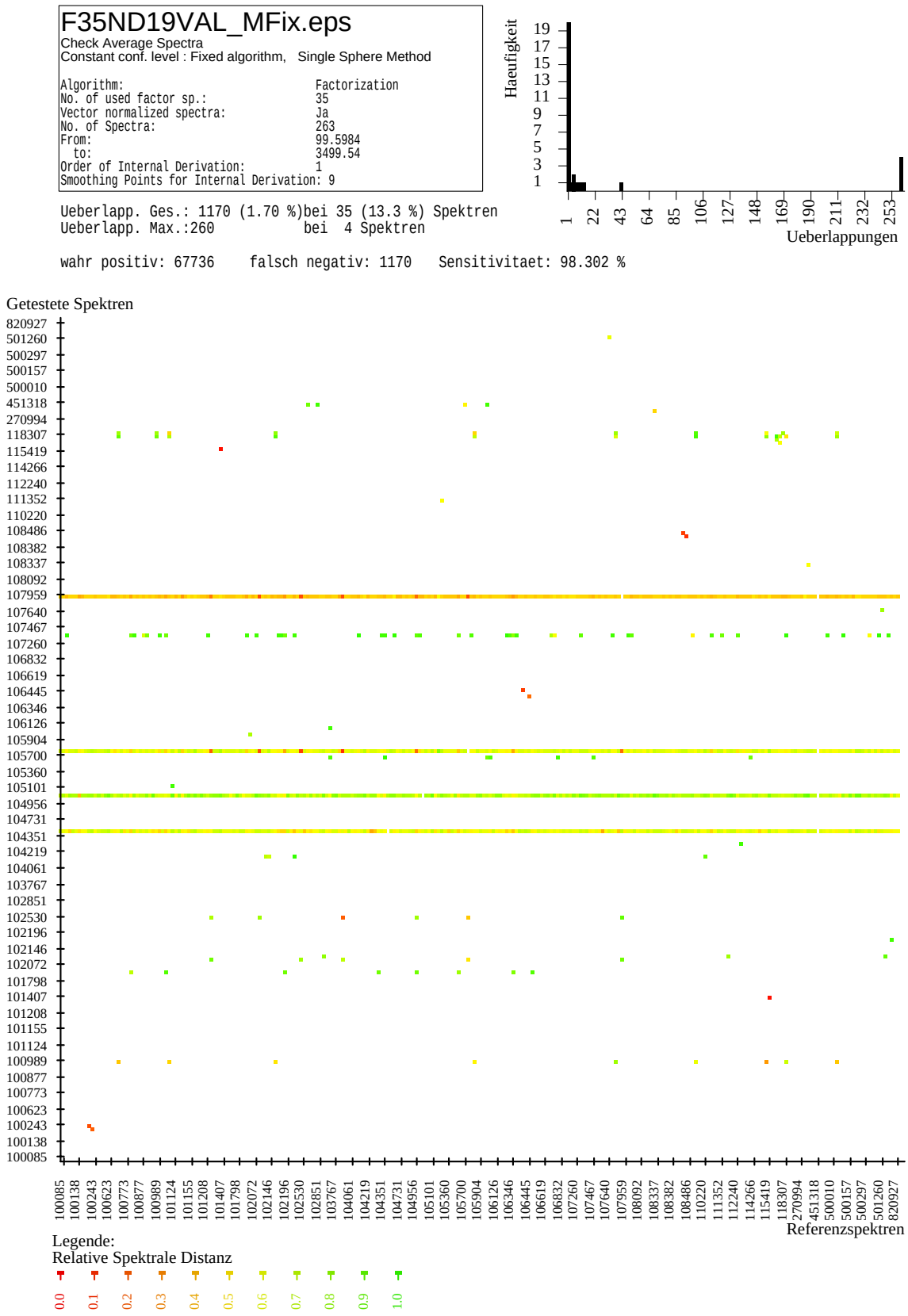


Abb. R15: Faktormethode (35 Faktoren, Vektornormierung, 1. Ableitung).

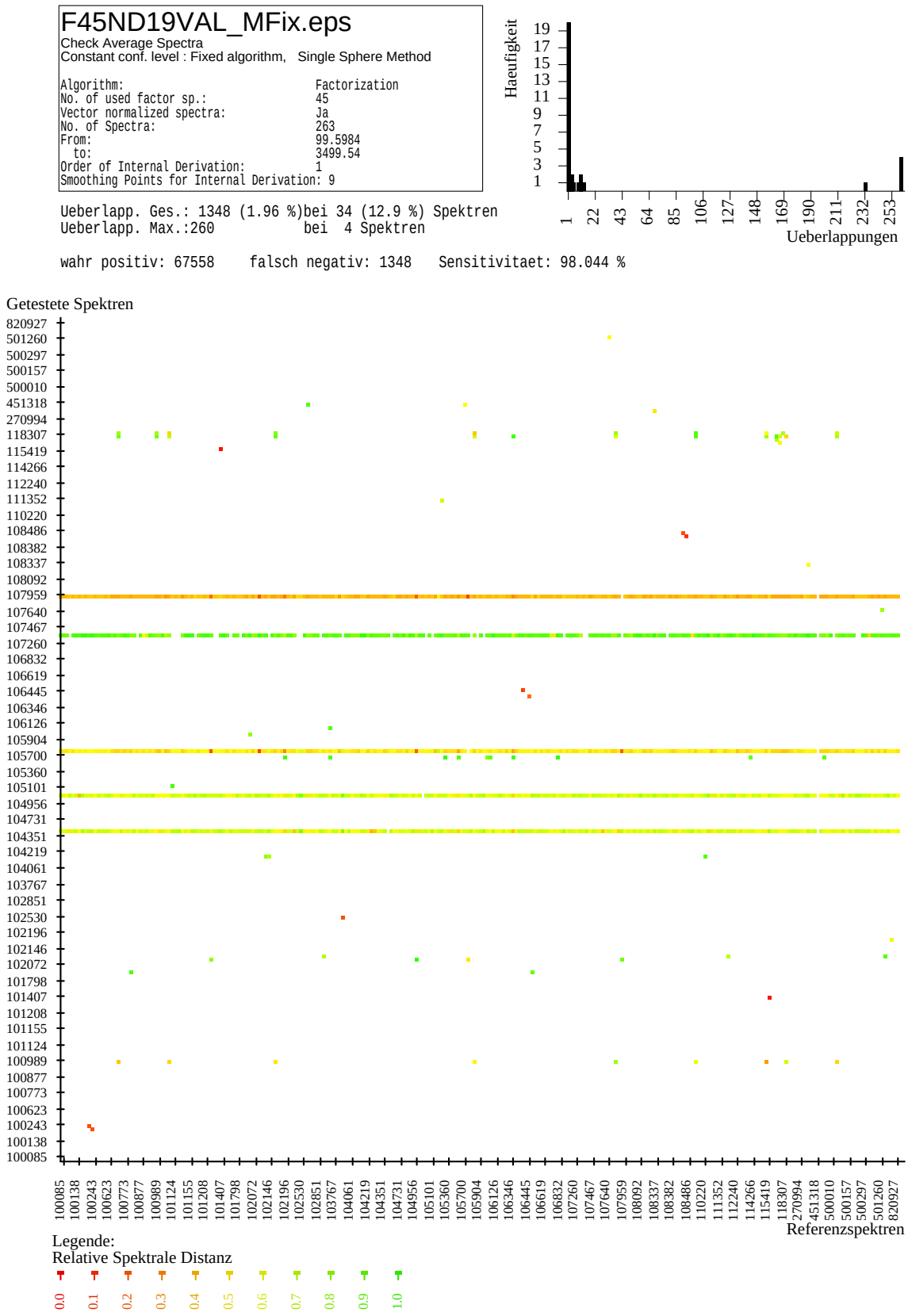


Abb. R16: Faktormethode (45 Faktoren, Vektornormierung, 1. Ableitung).

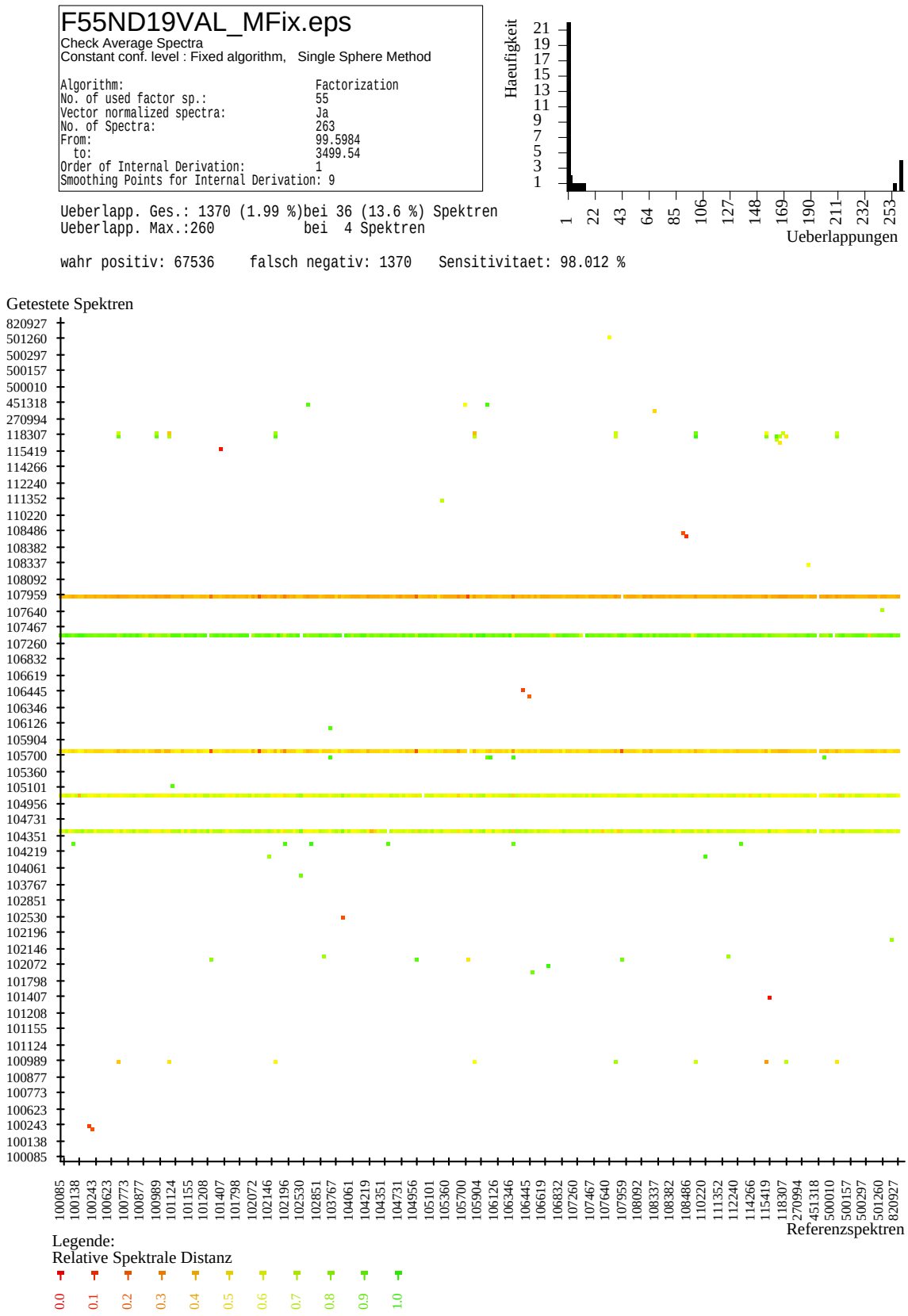


Abb. R17: Faktormethode (55 Faktoren, Vektornormierung, 1. Ableitung).

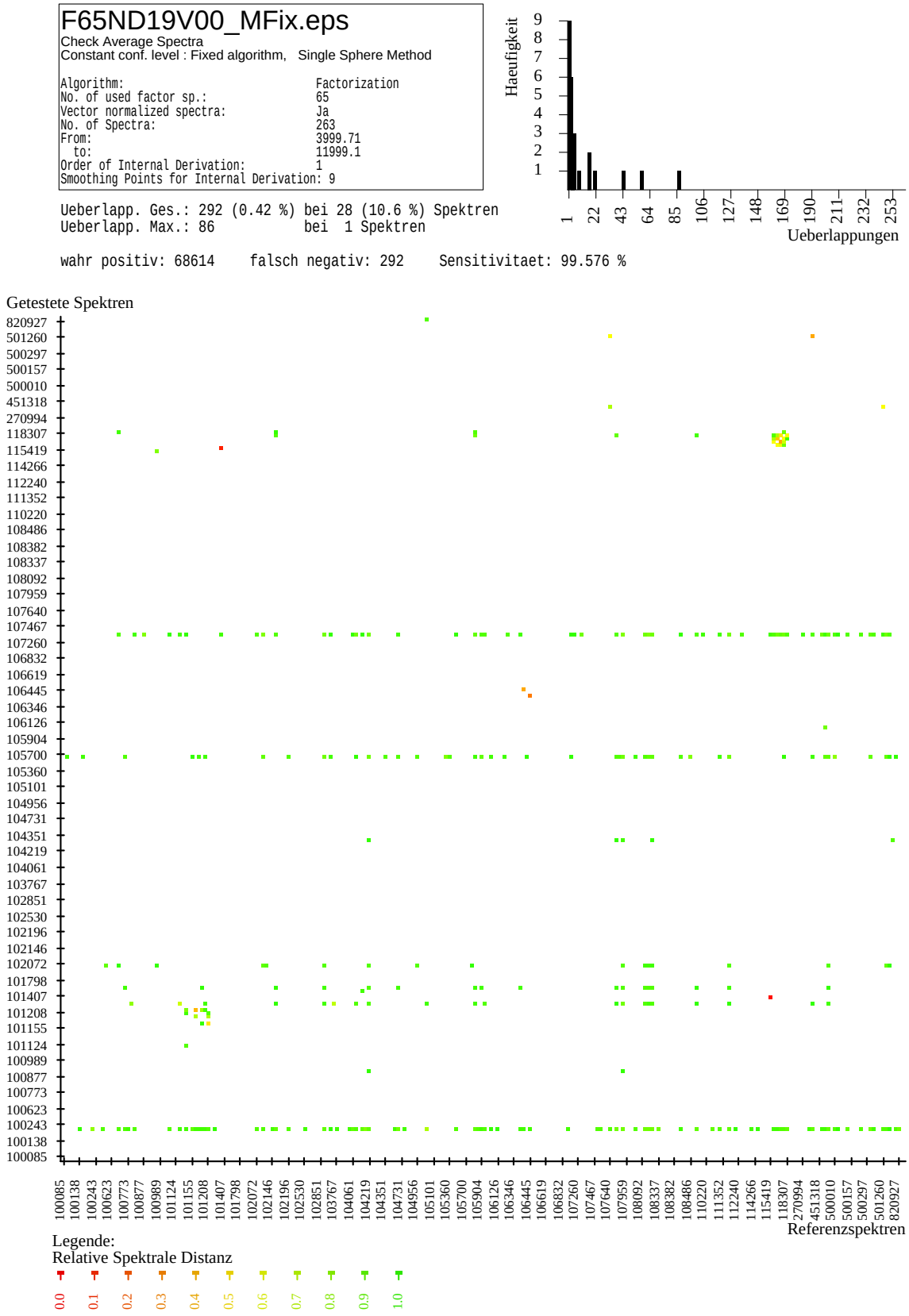


Abb. R18: Faktormethode (65 Faktoren, Vektornormierung, 1. Ableitung).

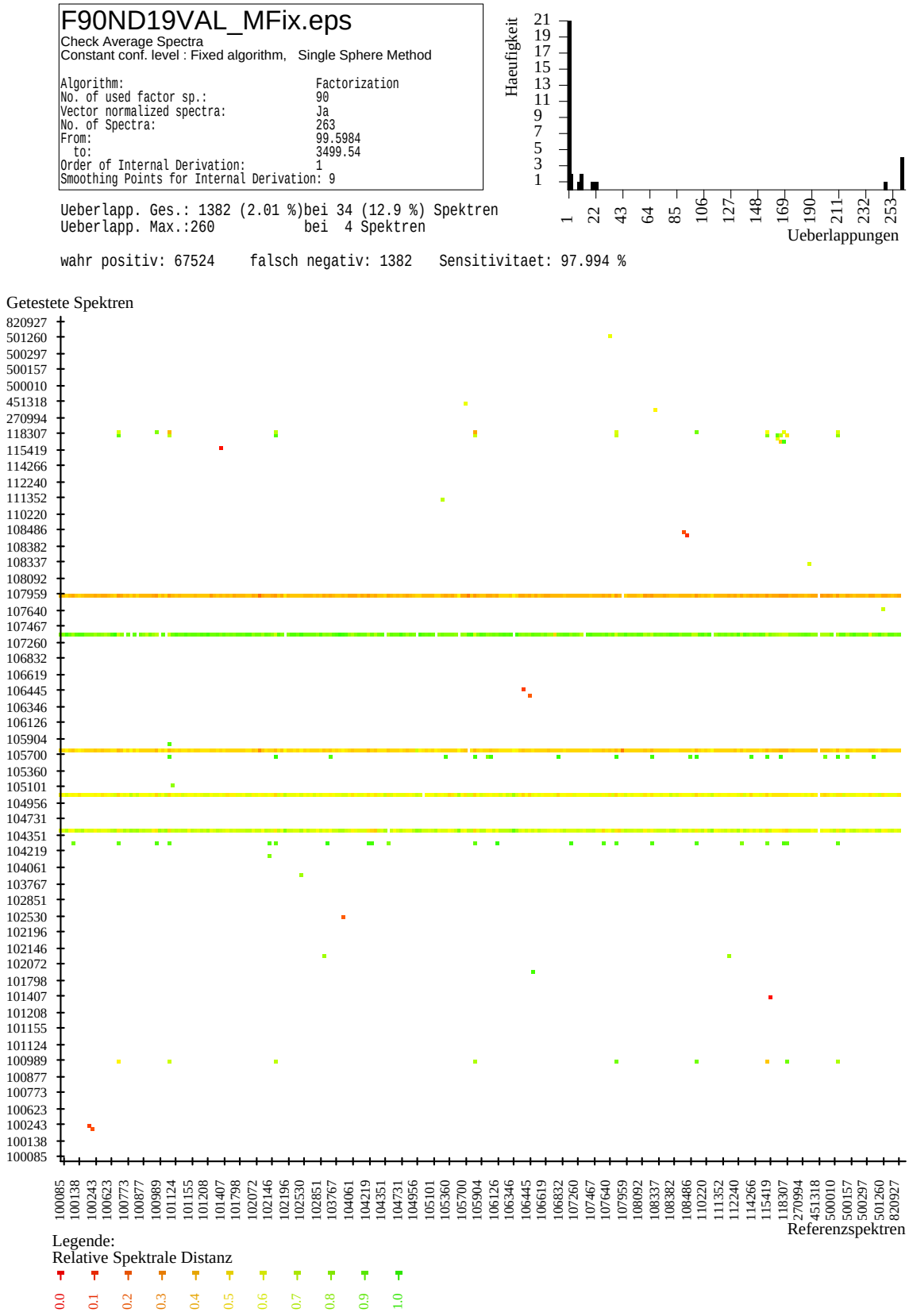


Abb. R19: Faktormethode (90 Faktoren, Vektornormierung, 1. Ableitung).

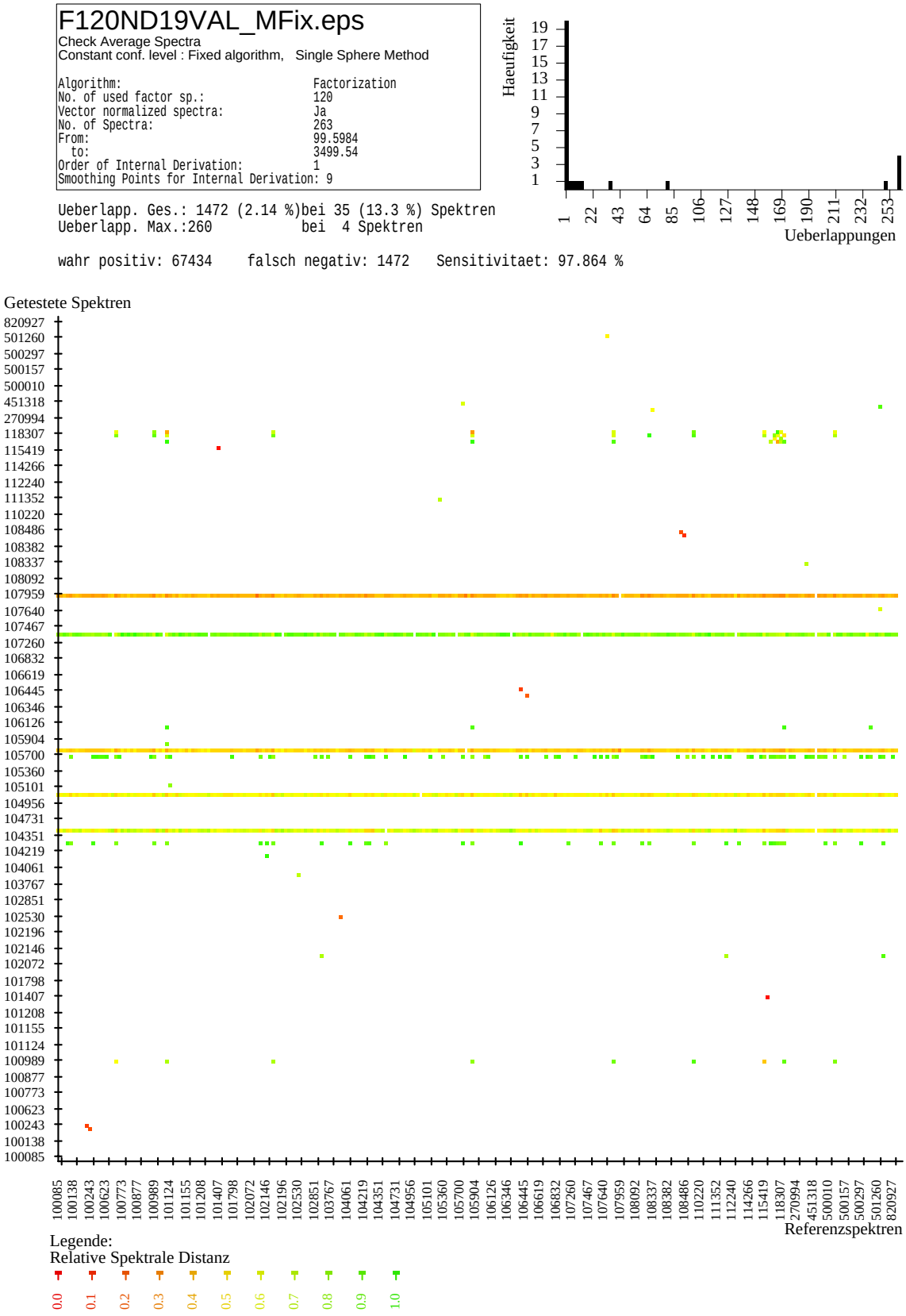


Abb. R20: Faktormethode (120 Faktoren, Vektornormierung, 1. Ableitung).

7.4.7 Raman, Variation des Spektralbereiches

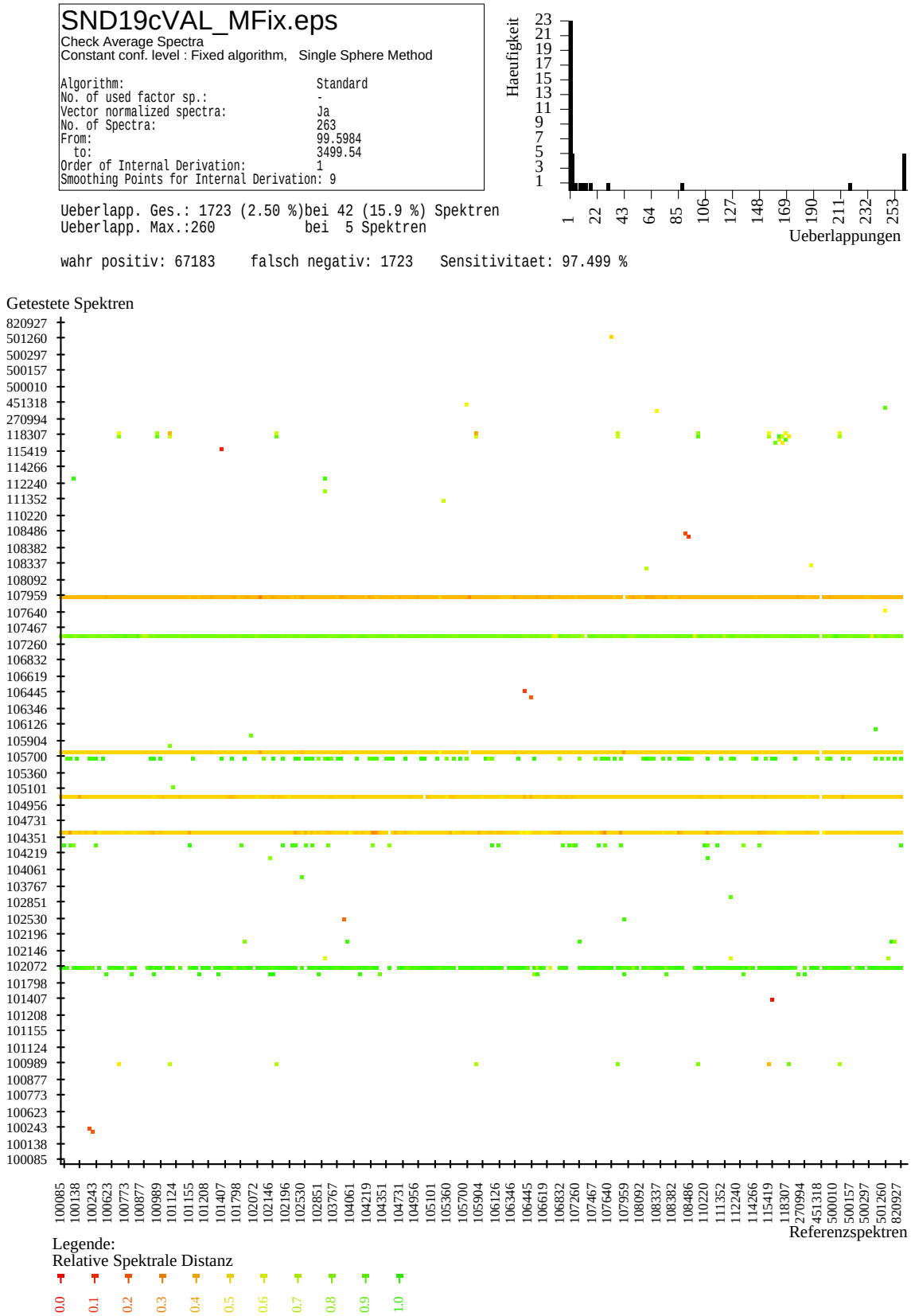


Abb. R21: Standardmethode (Vektornormierung, 1. Ableitung, 3500 cm^{-1} bis 100 cm^{-1}).

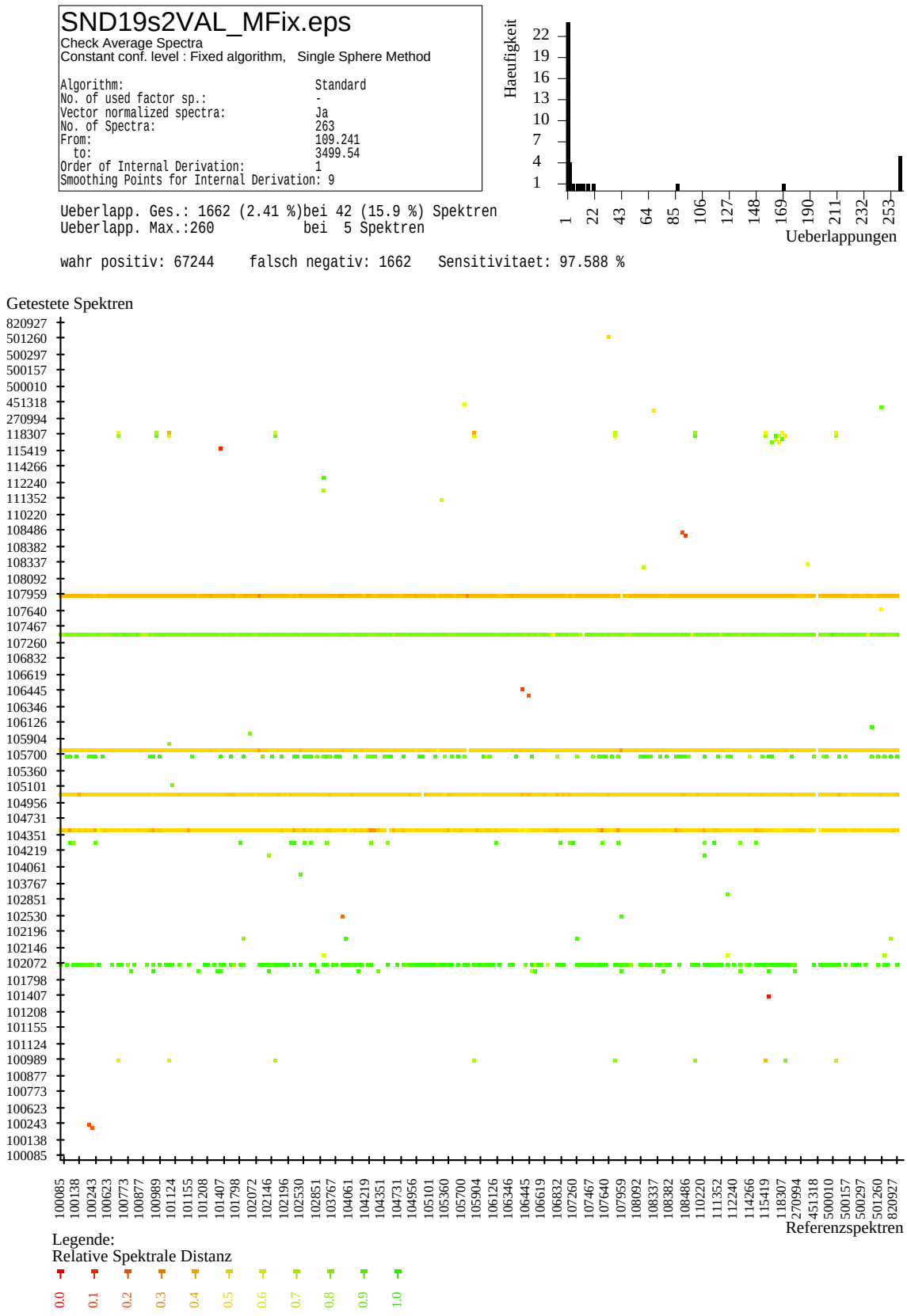


Abb. R22: Standardmethode (Vektornormierung, 1. Ableitung, 3500 cm^{-1} bis 110 cm^{-1}).

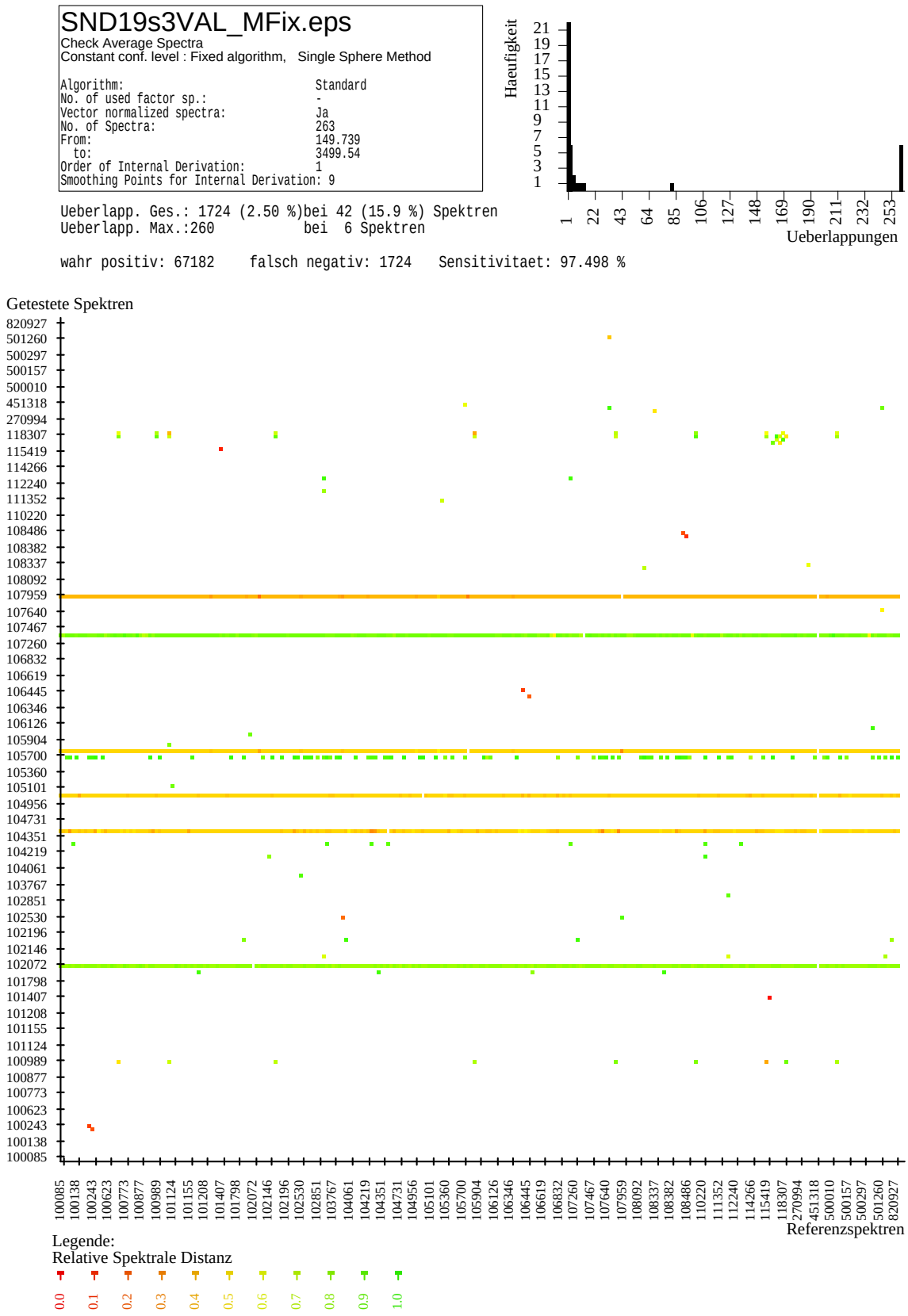


Abb. R23: Standardmethode (Vektornormierung, 1. Ableitung, 3500 cm^{-1} bis 150 cm^{-1}).

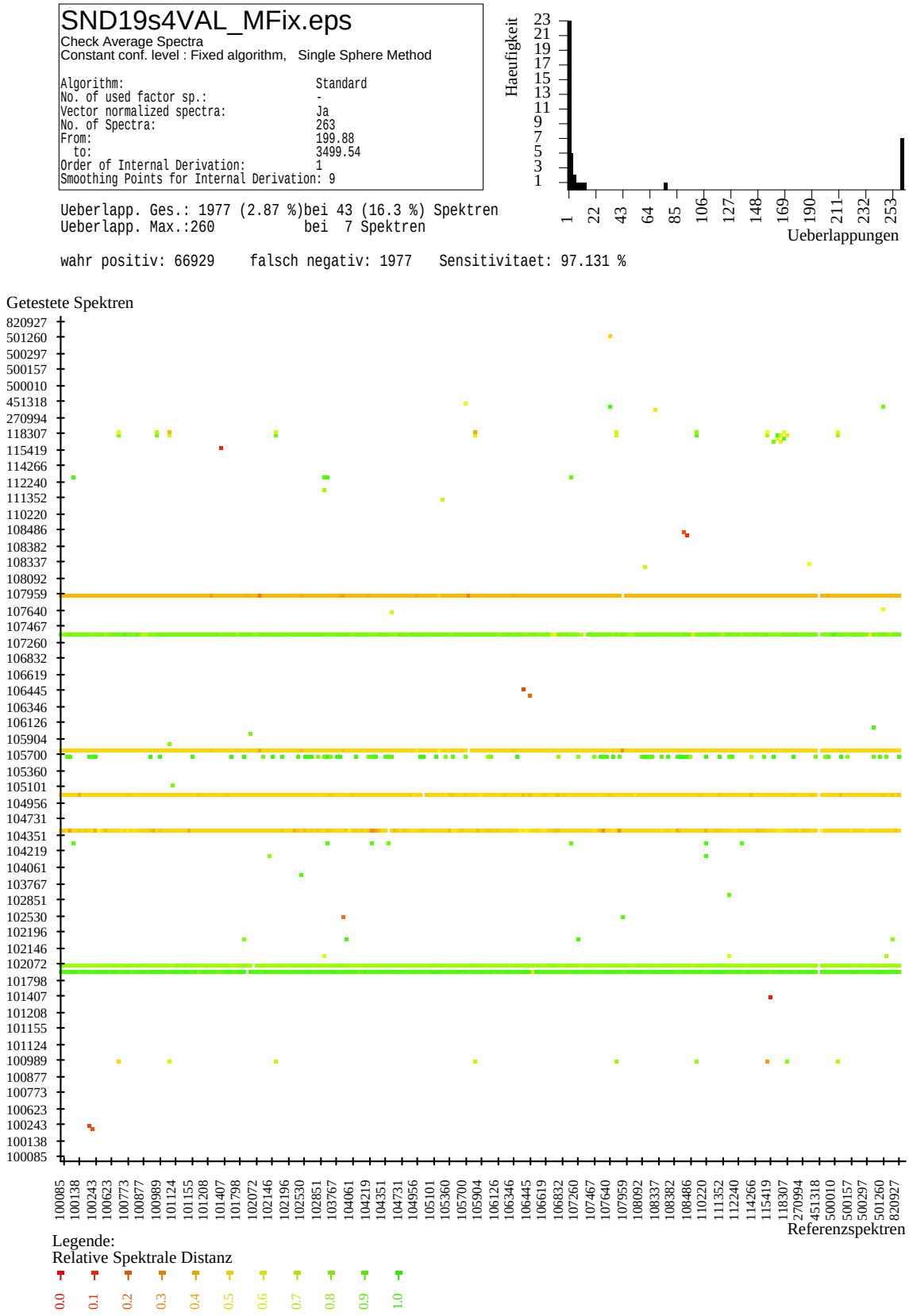


Abb. R24: Standardmethode (Vektornormierung, 1. Ableitung, 3500 cm^{-1} bis 200 cm^{-1}).

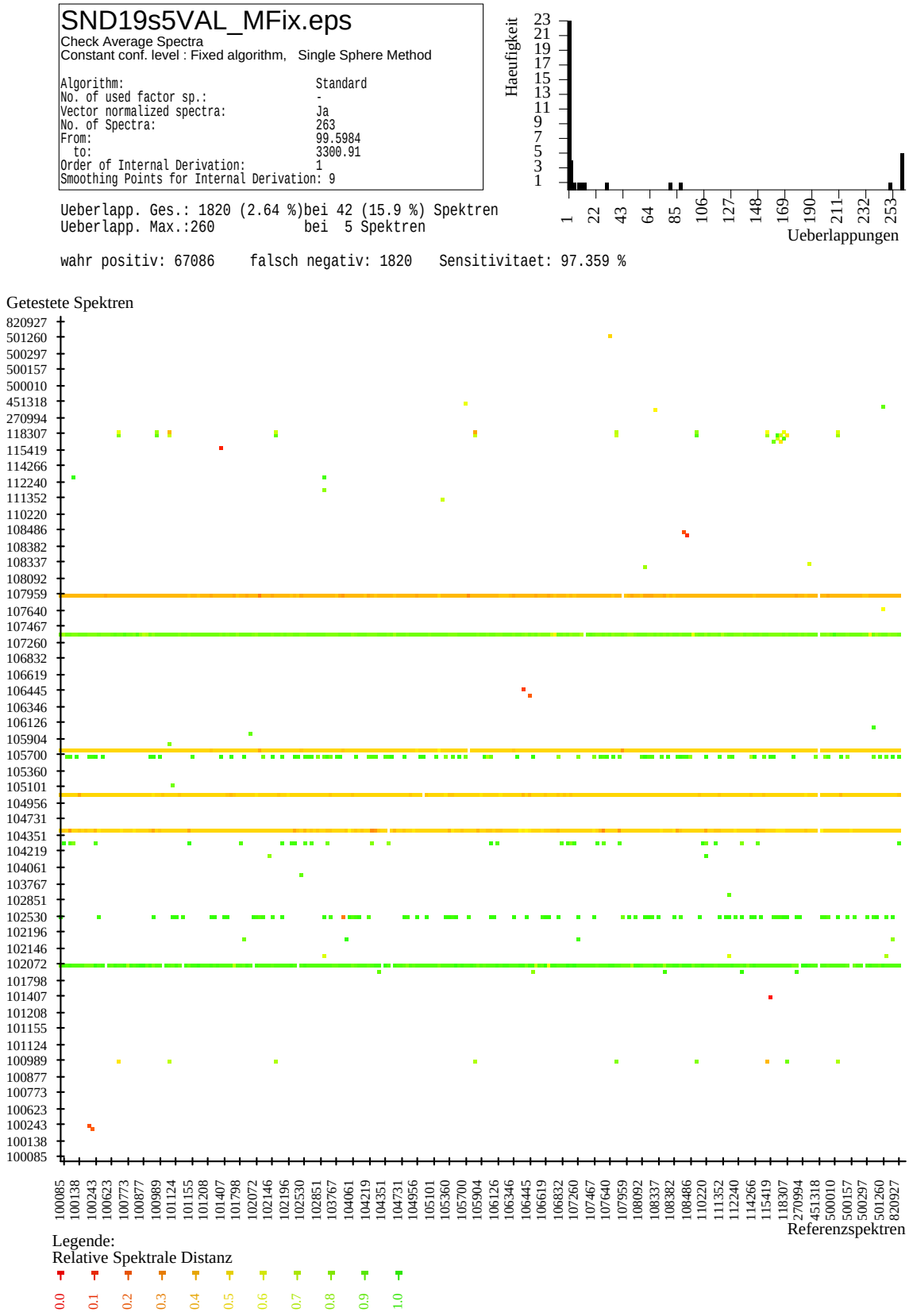


Abb. R25: Standardmethode (Vektornormierung, 1. Ableitung, 3300 cm^{-1} bis 100 cm^{-1}).

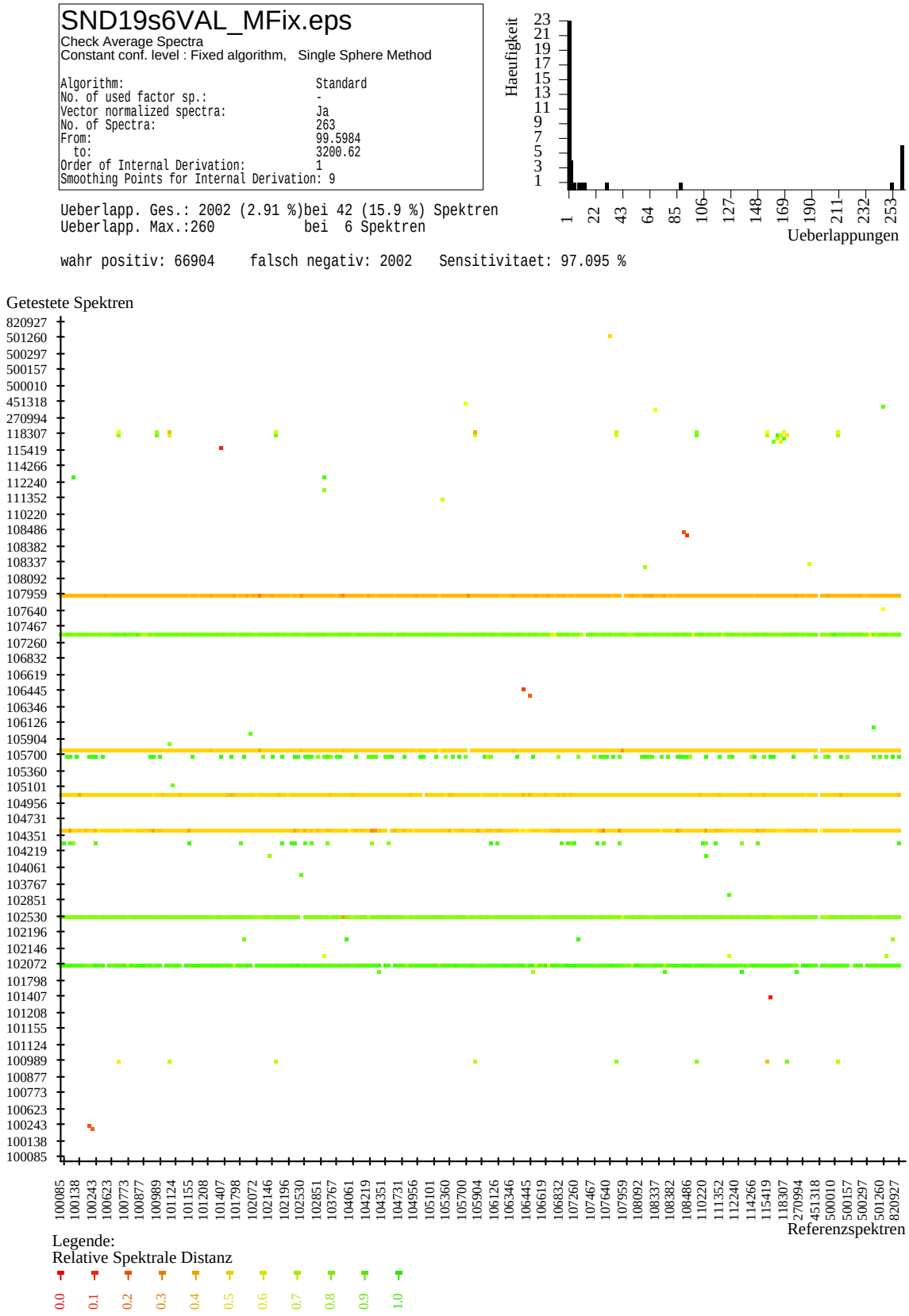


Abb. R26: Standardmethode (Vektornormierung, 1. Ableitung, 3200 cm^{-1} bis 100 cm^{-1})

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

7.4.8 Raman-Binärstrings

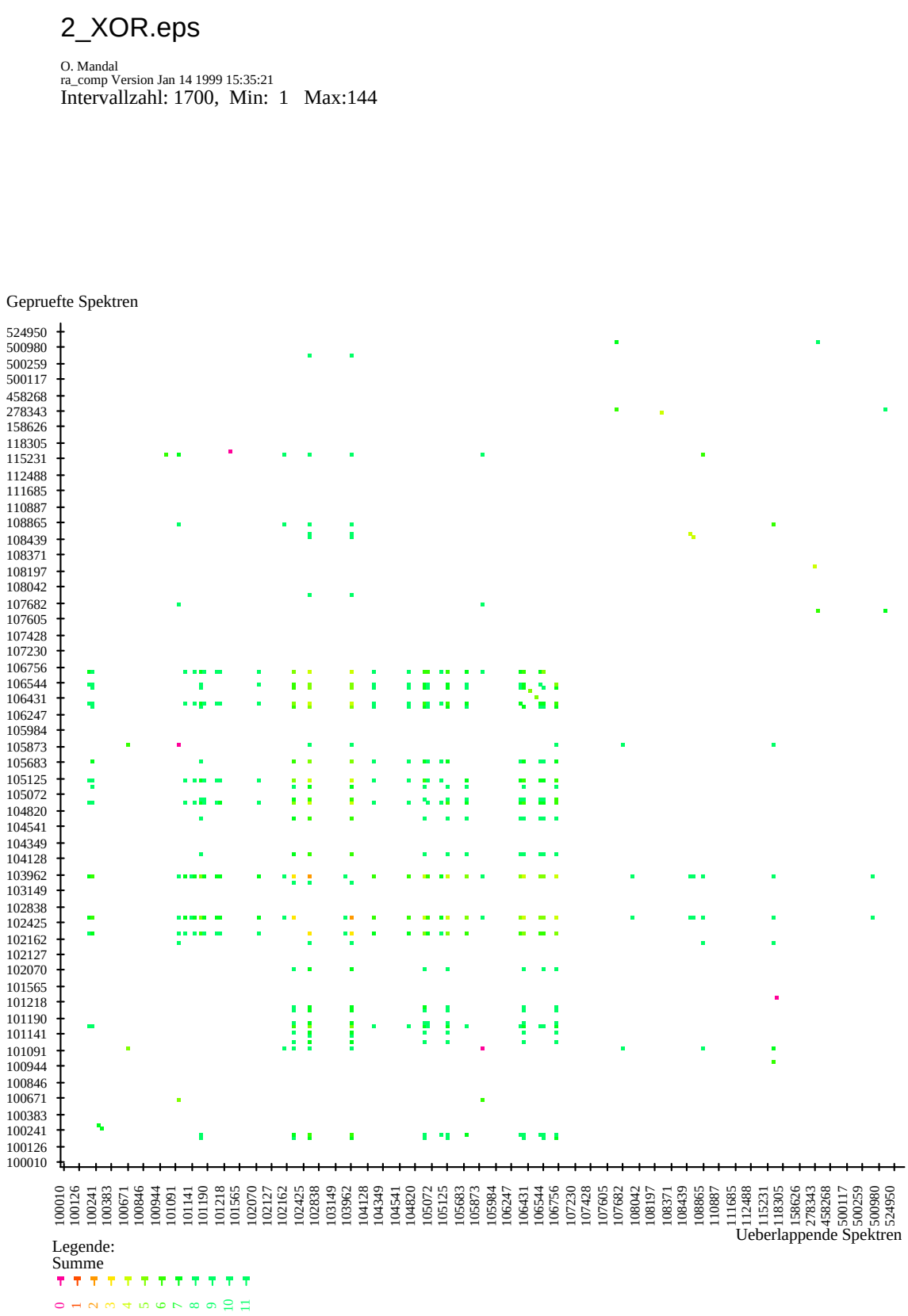


Abb. B1: Raman-Binärstring (2 cm^{-1}).

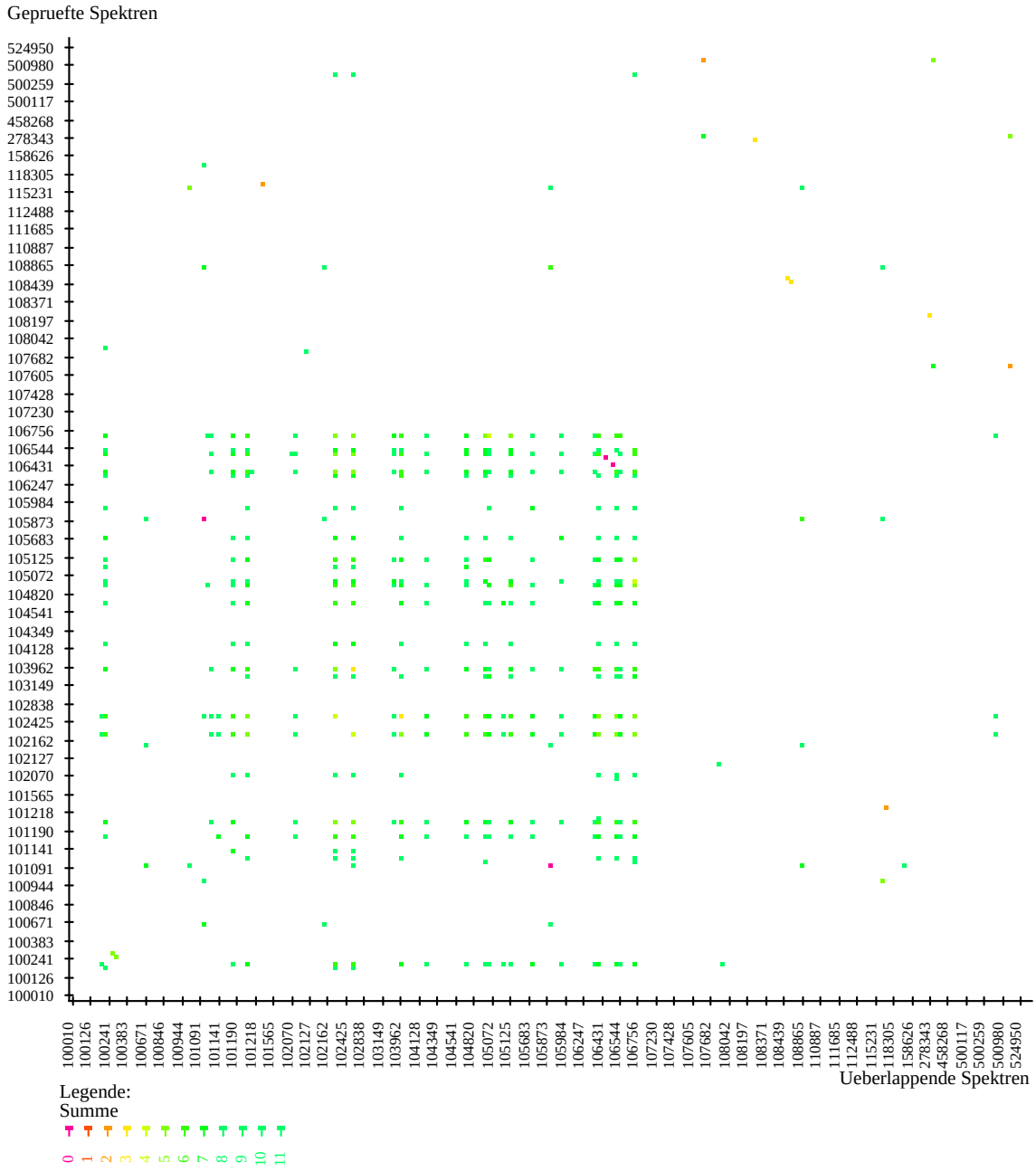


Abb. B2: NIR/Raman-Binärstring (5 cm^{-1}).

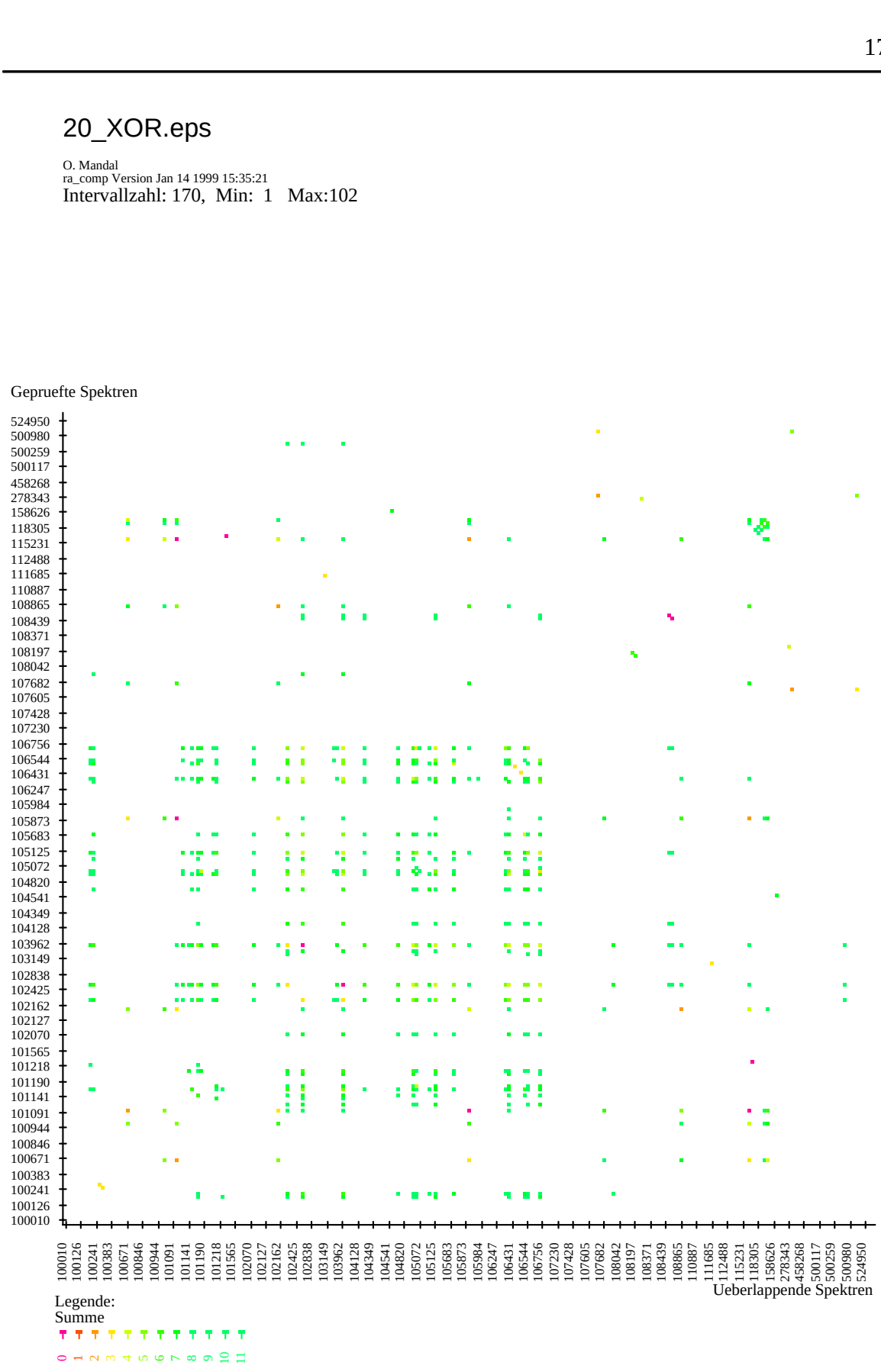


Abb. B3: Raman-Binärstring (20 cm^{-1}).

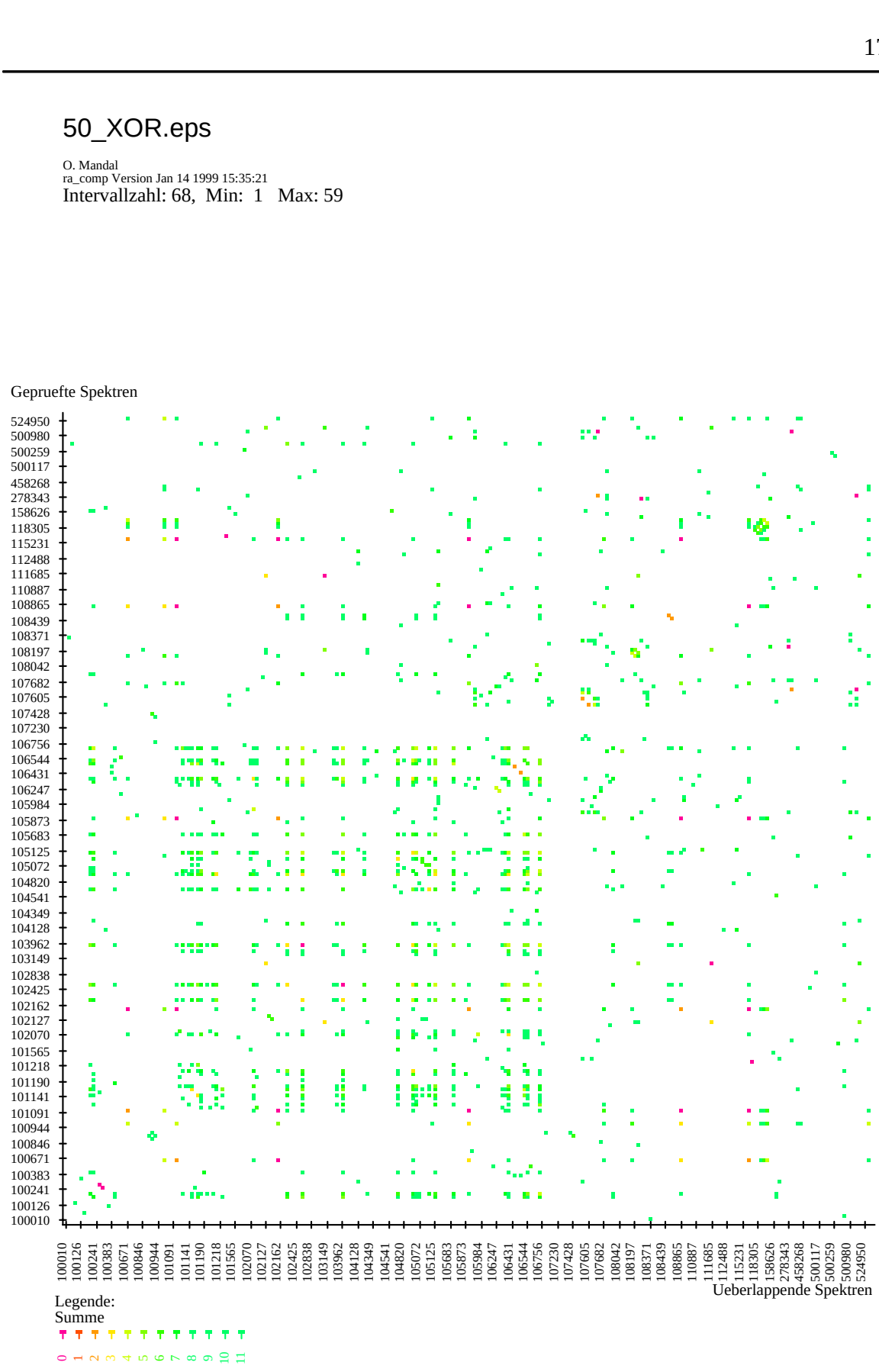


Abb. B4: Raman-Binärstring (50 cm^{-1}).

7.4.9 NIR-Binärstrings

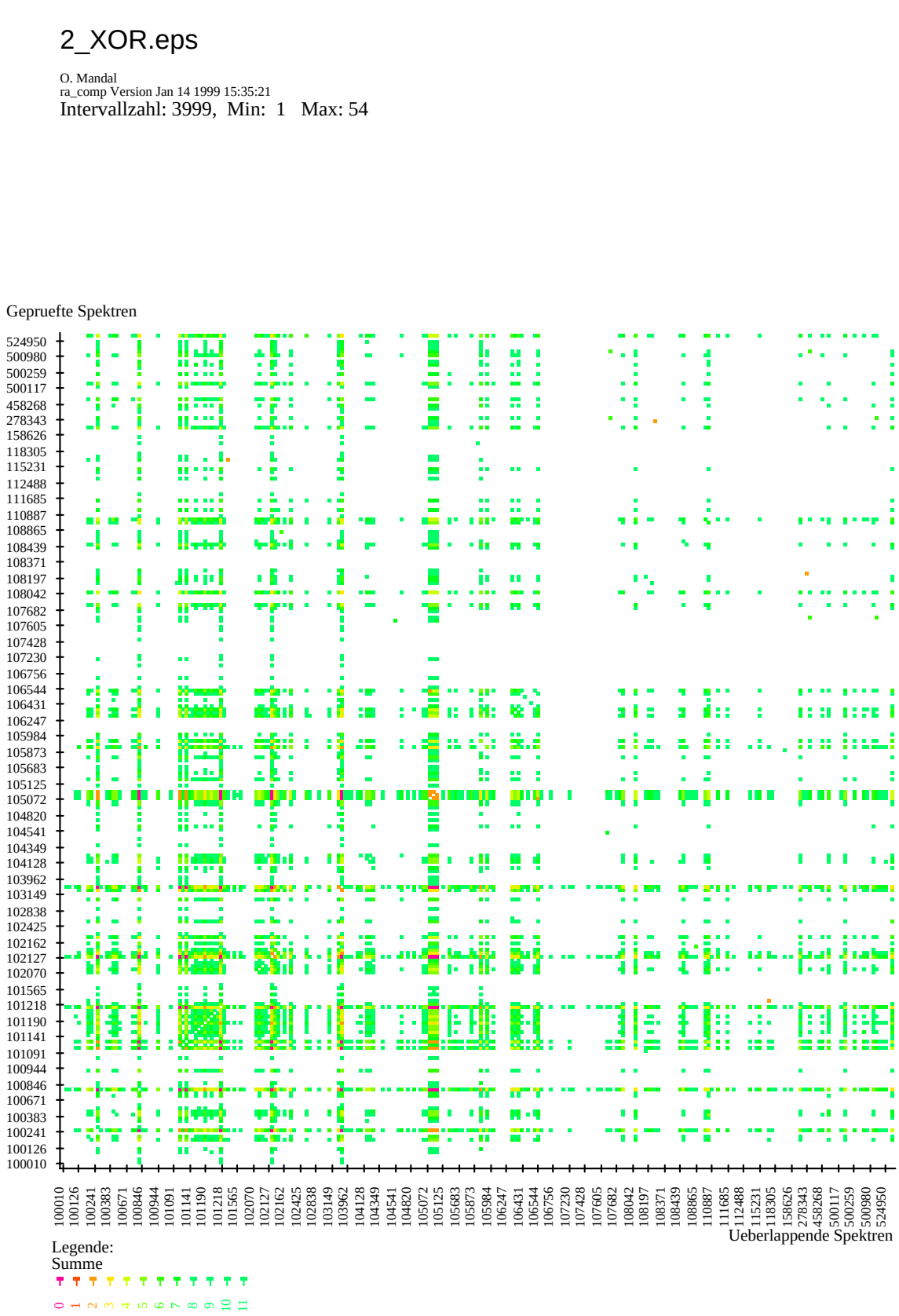


Abb. B5: NIR-Binärstring (2 cm^{-1}).

20_XOR.eps

O. Mandal
ra_comp Version Jan 14 1999 15:35:21
Intervallzahl: 399, Min: 1 Max: 50

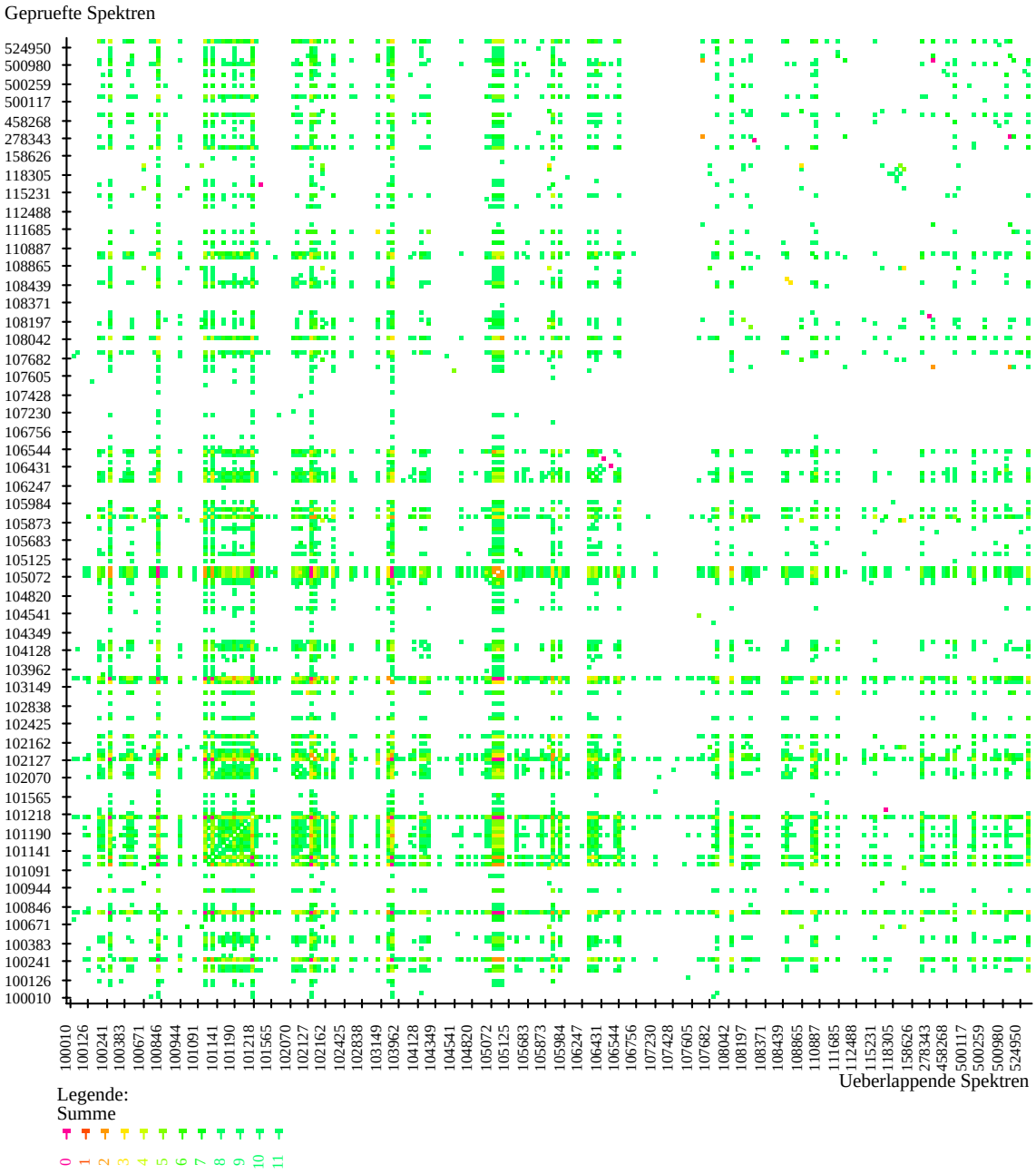


Abb. B6: NIR-Binärstring (20 cm^{-1}).

50_XOR.eps

O. Mandal
ra_comp Version Jan 14 1999 15:35:21
Intervallzahl: 159, Min: 1 Max: 39

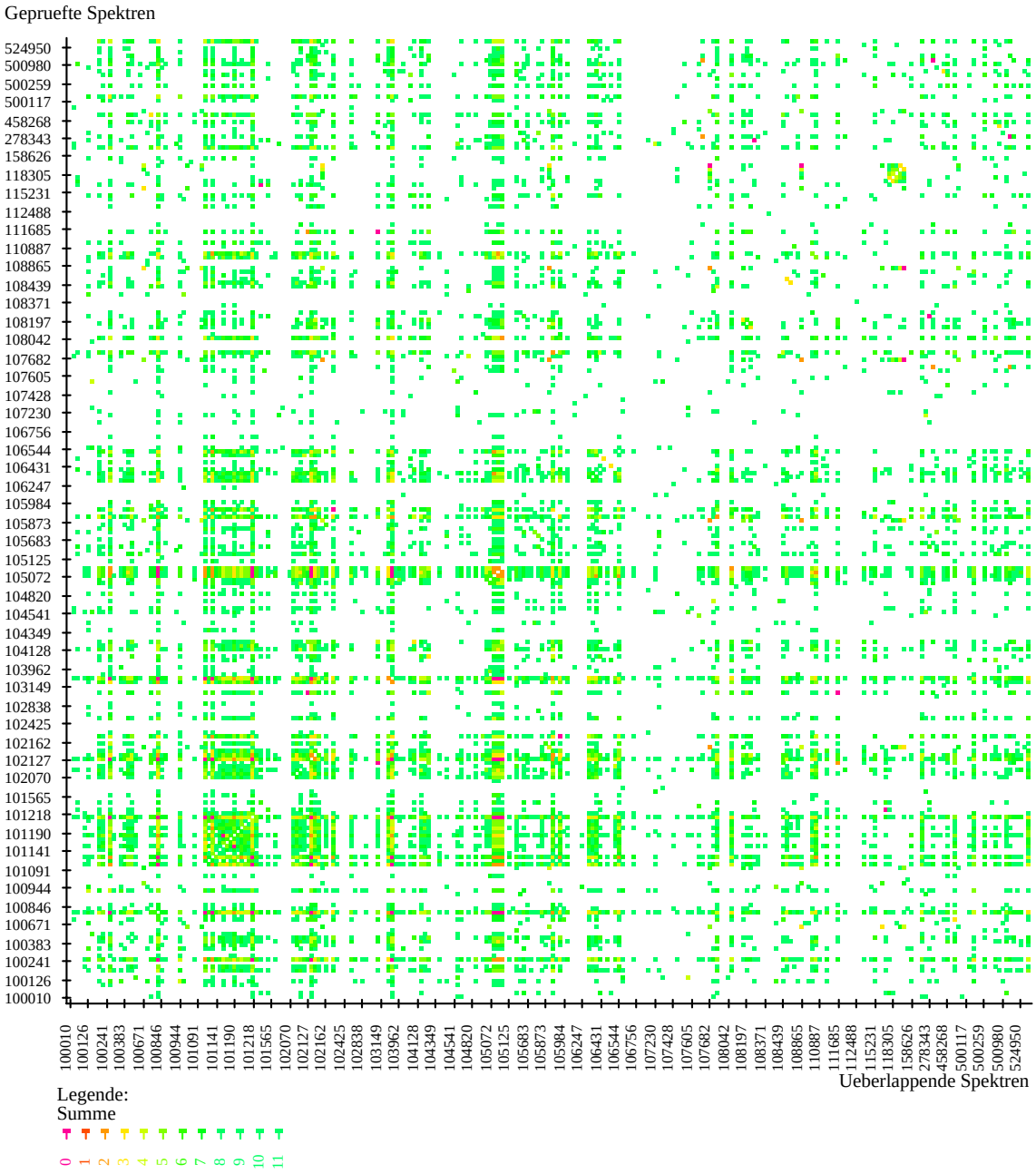


Abb. B7: NIR-Binärstring (50 cm^{-1}).

7.4.10 Kombinierte NIR/Raman-Binärstrings

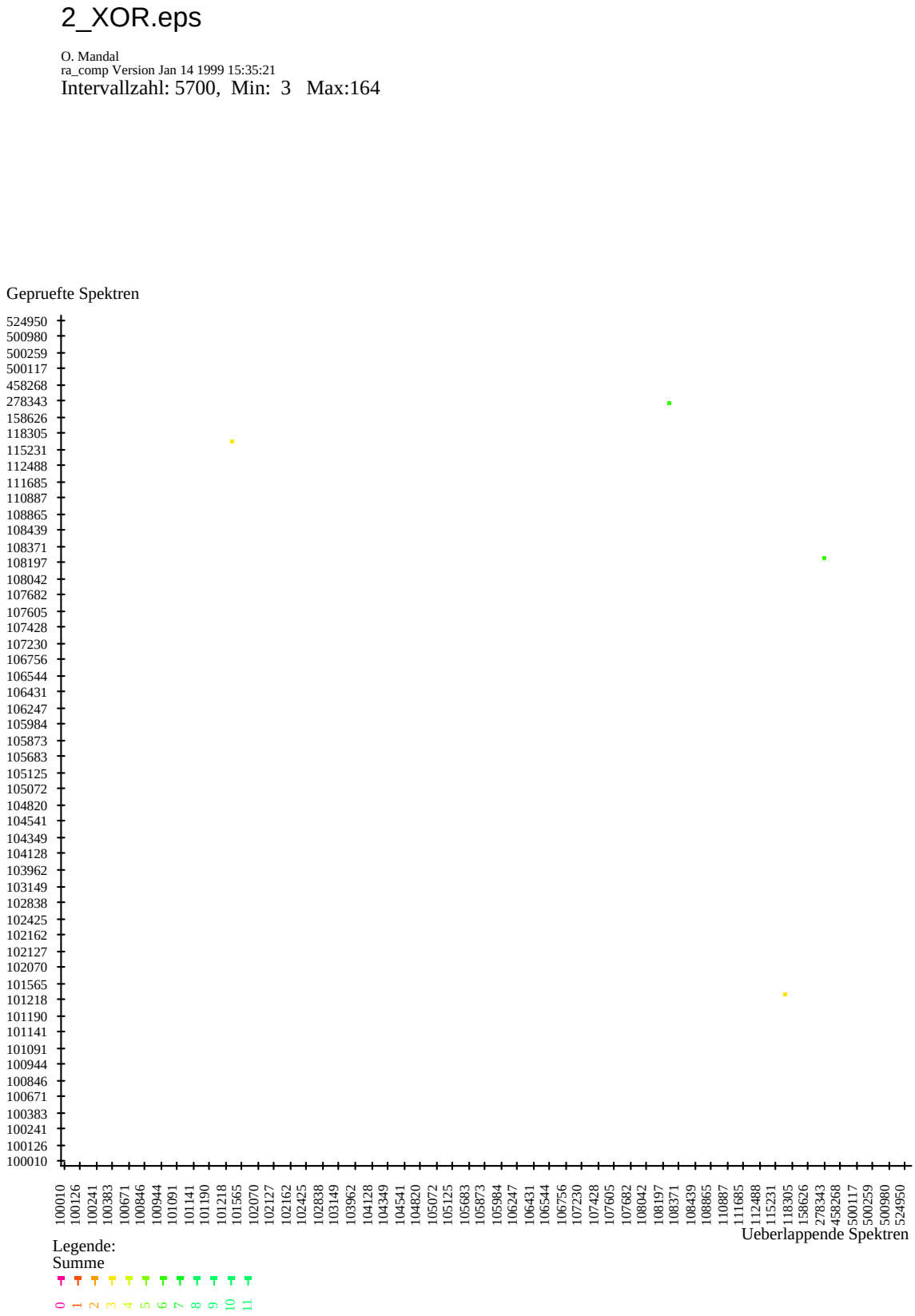


Abb. B8: NIR/Raman-Binärstring (2 cm^{-1}).

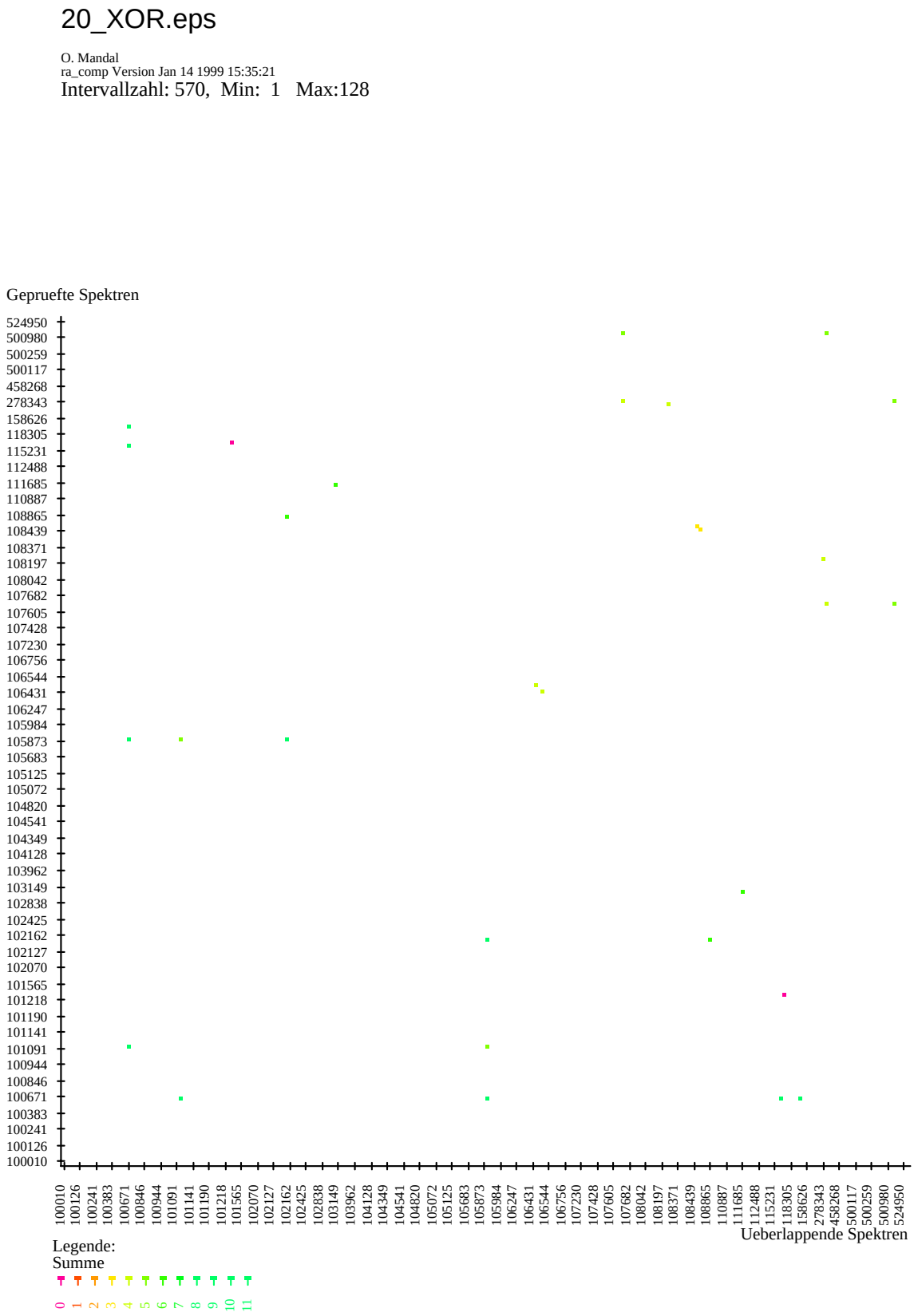


Abb. B9: NIR/Raman-Binärstring (20 cm^{-1}).

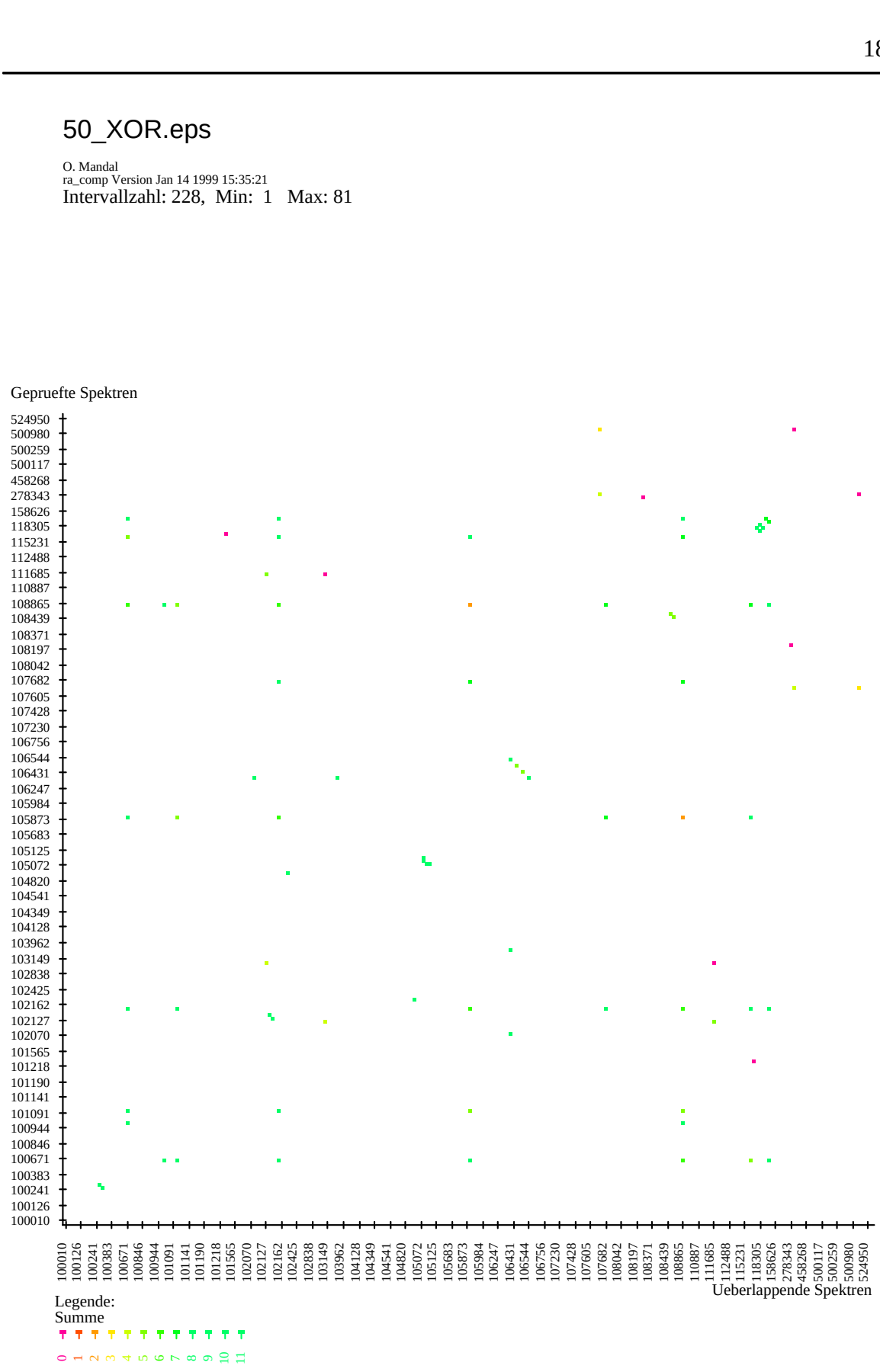


Abb. B10: NIR/Raman-Binärstring (50 cm^{-1}).