Validation Report

File name:	IDENT-capsules.FAA
Path:	S:\NIR\Documents\NIR-Projekte\Doktorarbeit\KAP\Model
Stored (date; time):	25/08/2019; 18:38:41
Operator name:	Admin
Library:	All
Sub libraries:	clear gelatin L-M
	clear gelatin MCC
	opaque hypromellose
	opaque gelatin L-M
	opaque gelatin MCC
	clear gelatin M_C-S
	clear gelatin L_C-S
	clear gelatin MCC_C-S
	opaque hypromellose M
	opaque hypromellose L
	opaque hypromellose MCC
	opaque gelatin M_C-S
	opaque hypromellose L_C-S
	opaque hypromellose MCC_C-S
Always use lowest IP level:	Yes

Parameters of library All:

Algorithm:	Factorization, 2 Factors (2,4)
Vector normalized spectra:	Yes
From:	8984
to:	4000
Order of Internal Derivative:	0
Smoothing Points for Internal Derivative:	1

Eigen-Values (not used ones are set to <0):

-21.4657
0.429027
-0.060608
0.0320879
-0.0121461
-0.000170742
-8.39058e-005
-5.68029e-005
-3.0922e-005
-1.58886e-005

-7.61689e-006
-5.70391e-006
-3.52958e-006
-3.04051e-006
-1.4167e-006
-9.24445e-007
-6.23477e-007
-2.29827e-007
-1.10446e-007
-6.32475e-008
-5.12545e-008
-2.46112e-008

Parameters of library clear gelatin L-M:

Algorithm:	Factorization, 2 Factors (2,3)
Vector normalized spectra:	Yes
From:	5100
to:	4800
Order of Internal Derivative:	2
Smoothing Points for Internal Derivative:	25

Eigen-Values (not used ones are set to <0):

-5.56888
0.428441
0.00240366
-0.000213226
-5.4059e-005
-1.17393e-005

Parameters of library clear gelatin M_C-S:

Algorithm:	Factorization, 1 Factors (2)
Vector normalized spectra:	Yes
From:	5700
to:	5620
From:	5480
to:	5400
From:	5256
to:	4800
Order of Internal Derivative:	2
Smoothing Points for Internal Derivative:	13

Eigen-Values (not used ones are set to <0):

-1.99975

0.000253682

Parameters of library clear gelatin L_C-S:

Algorithm:	Factorization, 1 Factors (2)
Vector normalized spectra:	Yes
From:	7260
to:	6900
From:	5720
to:	5620
From:	5580
to:	5420
Order of Internal Derivative:	2
Smoothing Points for Internal Derivative:	17

Eigen-Values (not used ones are set to <0):

-1.99932
0.000683262

Parameters of library clear gelatin MCC:

Algorithm:	Factorization, 1 Factors (2)
Vector normalized spectra:	Yes
From:	4800
to:	5100
Order of Internal Derivative:	2
Smoothing Points for Internal Derivative:	13

Eigen-Values (not used ones are set to <0):

-2.99606
0.00381202
-0.000132665

Parameters of library clear gelatin MCC_C-S:

Algorithm:	Factorization, 1 Factors (2)
Vector normalized spectra:	Yes
From:	5900
to:	5800
From:	5700
to:	5620
From:	5480
to:	5400
Order of Internal Derivative:	1
Smoothing Points for Internal Derivative:	13

Eigen-Values (not used ones are set to <0):
-1.99976
0.000242158

Parameters of library opaque hypromellose:

Algorithm:	Factorization, 1 Factors (2)
Vector normalized spectra:	Yes
From:	7284
to:	6092
Order of Internal Derivative:	1
Smoothing Points for Internal Derivative:	17

Eigen-Values (not used ones are set to <0):
-7.7612
0.188298
-0.0499955
-0.000424639
-6.69406e-005
-1.37275e-005
-3.88629e-006
-8.84254e-007

Parameters of library opaque hypromellose M:

Algorithm:	Factorization, 1 Factors (2)
Vector normalized spectra:	Yes
From:	7272
to:	6560
From:	5480
to:	5400
From:	5272
to:	4864
Order of Internal Derivative:	2
Smoothing Points for Internal Derivative:	5

Eigen-Values (not used ones are set to <0):
-1.99799
0.0020097

Parameters of library opaque hypromellose L:

Algorithm:	Factorization, 1 Factors (2)
Vector normalized spectra:	Yes

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        From:                                   4900
          to:                                   4960
        Order of Internal Derivative:           2
        Smoothing Points for Internal Derivative: 5

        Eigen-Values (not used ones are set to <0):
                                                -2.87033
                                                0.129334
                                                -0.000340131


Parameters of library opaque hypromellose L_C-S:
        Algorithm:                              Factorization, 1 Factors (2)
        Vector normalized spectra:              Yes
        From:                                   7272
          to:                                   6900
        From:                                   5480
          to:                                   5400
        From:                                   5272
          to:                                   5100
        Order of Internal Derivative:           2
        Smoothing Points for Internal Derivative: 5

        Eigen-Values (not used ones are set to <0):
                                                -1.99811
                                                0.00188931


Parameters of library opaque hypromellose MCC:
        Algorithm:                              Factorization, 1 Factors (2)
        Vector normalized spectra:              Yes
        From:                                   6052
          to:                                   6000
        From:                                   4972
          to:                                   4900
        Order of Internal Derivative:           2
        Smoothing Points for Internal Derivative: 5

        Eigen-Values (not used ones are set to <0):
                                                -2.88204
                                                0.114744
                                                -0.00321113


Parameters of library opaque hypromellose MCC_C-S:
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Algorithm: Factorization, 1 Factors (2)
Vector normalized spectra: Yes
From: 5900
to: 5800
From: 5700
to: 5620
From: 5480
to: 5400
From: 5272
to: 4864
Order of Internal Derivative: 2
Smoothing Points for Internal Derivative: 25

Eigen-Values (not used ones are set to <0):
-1.99928
0.000723985

Parameters of library opaque gelatin L-M:
Algorithm: Factorization, 1 Factors (1)
Vector normalized spectra: Yes
From: 4800
to: 5100
Order of Internal Derivative: 2
Smoothing Points for Internal Derivative: 21

Parameters of library opaque gelatin M_C-S:
Algorithm: Factorization, 1 Factors (2)
Vector normalized spectra: Yes
From: 7780
to: 7032
Order of Internal Derivative: 2
Smoothing Points for Internal Derivative: 9

Eigen-Values (not used ones are set to <0):
-1.99657
0.00342605

Parameters of library opaque gelatin MCC:
Algorithm: Factorization, 1 Factors (2)
Vector normalized spectra: Yes
From: 5100
to: 4800

Order of Internal Derivative: 2
Smoothing Points for Internal Derivative: 25

Eigen-Values (not used ones are set to <0):
-1.99926
0.000741372

Check Original Spectra
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Spectra from the following groups are outside:

Group Name (Threshold)	Not Identified (Distance)	Final Sub Library
clear gelatin/lactose/S	Sildenafil 2 mg Gelatine Lactose 128 8_S25-01_Probe 2_klar_1_Lactose_009_20170529_162105.001	IP3: clear gelatin L_C-S
(0.732509)	(1.090309)	
opaque gelatin/mannitol/S	Sildenafil 2 mg Gelatine Lactose 128 8_S02A-01__wei+ƒ_1_Mannitol_007_20170531_125921.001	IP3: opaque gelatin M_C-S
(0.497402)	(0.724150)	
clear gelatin/lactose/C	Captopril 2 mg Stabi_C25-02_1_HGK (klar)_1_L-A_005_20170523_183054.001	IP3: clear gelatin L_C-S
(0.505702)	(0.541848)	
opaque gelatin/mannitol/C	Captopril 2 mg Stabi_C31-02_1_HGK (wei+ƒ)_1_M-A_006_20170523_203121.001	IP3: opaque gelatin M_C-S
(0.911630)	(0.921687)	

Spectra from the following groups can be confused with other groups on the final (sub) libra
Groups which should be assigned to a new common sub-library are listed together:

Group Name	Final (Sub) Library
opaque gelatin/mannitol/S opaque gelatin/mannitol/C	IP3: opaque gelatin M_C-S

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Details:

Group Name	Confused (Distance)	With (Threshold)	Final (Sub) Library
opaque gelatin/mannitol/S	Sildenafil 2 mg Gelatine Lactose 128 8_S02A-01__wei+f_1_Mannitol_007_20170531_125921.001 (0.690063)	opaque gelatin/mannitol/C (0.911630)	IP3: opaque gelatin M_C
opaque gelatin/mannitol/C	Captopril 2 mg Stabi_C31-02_1_HGK (wei+f)_1_M-A_006_20170523_203121.001 (0.492527)	opaque gelatin/mannitol/S (0.497402)	IP3: opaque gelatin M_C

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Summary:

Original Spectra, which can be confused with other references: 2 of 902
Original Spectra, which are outside: 4 of 902
Original Spectra, which can be uniquely identified: 898 of 902
From following Groups, all Original Spectra can be uniquely identified:

clear gelatin/lactose/H	all in	IP2: clear gelatin L-M
clear gelatin/mannitol/C	all in	IP3: clear gelatin M_C-S
clear gelatin/mannitol/H	all in	IP2: clear gelatin L-M
clear gelatin/mannitol/S	all in	IP3: clear gelatin M_C-S
clear gelatin/MCC/C	all in	IP3: clear gelatin MCC_C-S

clear gelatin/MCC/H	all in	IP2: clear gelatin MCC
clear gelatin/MCC/S	all in	IP3: clear gelatin MCC_C-S
opaque gelatin/lactose/S	all in	IP2: opaque gelatin L-M
opaque gelatin/MCC/H	all in	IP2: opaque gelatin MCC
opaque gelatin/MCC/S	all in	IP2: opaque gelatin MCC
opaque hypromellose/lactose/C	all in	IP4: opaque hypromellose L_C-S
opaque hypromellose/lactose/H	all in	IP3: opaque hypromellose L
opaque hypromellose/lactose/S	all in	IP4: opaque hypromellose L_C-S
opaque hypromellose/mannitol/C	all in	IP3: opaque hypromellose M
opaque hypromellose/mannitol/S	all in	IP3: opaque hypromellose M
opaque hypromellose/MCC/C	all in	IP4: opaque hypromellose MCC_C-S
opaque hypromellose/MCC/H	all in	IP3: opaque hypromellose MCC
opaque hypromellose/MCC/S	all in	IP4: opaque hypromellose MCC_C-S