

Electronic Supporting Information (ESI) for

Multi-Layered Analyses Using Directed Partitioning to Identify and Discriminate between Biogenic Amines

Toby L. Nelson, Ivy Tran, Tim G. Ingallinera, Marc S. Maynor, and John J. Lavigne*

*Department of Chemistry and Biochemistry, University of South Carolina,
Columbia, South Carolina 29208;
E-mail: lavigne@mail.chem.sc.edu*

Single layered analysis: Polymer 1 sensor responding to all biogenic amines

Table S1. Group frequencies

BDA	HistA	PeDA	SperM	SpermD	TryptA	TyrA
84	84	84	84	84	84	84

Table S2. Group means

	BDA	HistA	PeDA	SperM	SpermD	TryptA	TyrA
VAR00002	0.015	0.015	0.016	0.018	0.018	0.015	0.015
VAR00003	0.022	0.022	0.024	0.023	0.025	0.022	0.022
VAR00004	0.030	0.029	0.030	0.028	0.029	0.029	0.029
VAR00005	0.029	0.029	0.029	0.027	0.028	0.028	0.028
VAR00006	0.019	0.020	0.019	0.018	0.018	0.019	0.019
VAR00007	0.009	0.010	0.009	0.008	0.008	0.010	0.010
VAR00008	0.004	0.004	0.003	0.004	0.003	0.004	0.004
VAR00009	0.001	0.001	0.001	0.004	0.002	0.002	0.002
VAR00010	0.001	0.001	0.001	0.003	0.002	0.001	0.002

Table S3. Between groups F-matrix -- df = 8 574

	BDA	HistA	PeDA	SperM	SpermD	TryptA	TyrA
BDA	0.000						
HistA	68.931	0.000					
PeDA	239.621	205.070	0.000				
SperM	1322.318	1132.778	731.542	0.000			
SpermD	1289.061	1119.781	557.256	108.470	0.000		
TryptA	73.435	71.446	163.465	1052.719	971.628	0.000	
TyrA	164.778	114.639	161.385	835.084	790.500	33.032	0.000

Wilks' lambda

Lambda = 0.0008 df = 8 6 581

Approx. F = 189.9052 df = 48 2828 prob = 0.0000

Table S4. Classification functions

	BDA	HistA	PeDA	SperM	SpermD	TryptA	TyrA
CONSTANT	-989624.648	-991605.439	-988760.439	-987364.104	-988367.205	-991699.594	-991191.671
VAR00002	6530334.383	6531402.299	6522092.763	6485045.491	6494977.758	6524046.891	6511041.855
VAR00003	2.20824E+07	2.21133E+07	2.20902E+07	2.21389E+07	2.21460E+07	2.21341E+07	2.21462E+07
VAR00004	7586394.463	7589037.869	7589834.705	7556527.471	7566879.140	7579261.578	7570005.539
VAR00005	2.38860E+07	2.39025E+07	2.38341E+07	2.37759E+07	2.37813E+07	2.39049E+07	2.38915E+07
VAR00006	1.00609E+07	1.00901E+07	1.01069E+07	1.01902E+07	1.01897E+07	1.00858E+07	1.01001E+07
VAR00007	1.96638E+07	1.96714E+07	1.96303E+07	1.95136E+07	1.95426E+07	1.96725E+07	1.96513E+07
VAR00008	1.57877E+07	1.57985E+07	1.57561E+07	1.58091E+07	1.57931E+07	1.58089E+07	1.58097E+07
VAR00009	0.000	0.000	0.000	0.000	0.000	0.000	0.000
VAR00010	3.53533E+07	3.53995E+07	3.53684E+07	3.53350E+07	3.53604E+07	3.53929E+07	3.53896E+07

Table S5.

Variable	F-to-remove	Tolerance	Variable	F-to-enter	Tolerance
2 VAR00002	47.69	0.082317	9 VAR00009	11.30	0.000977
3 VAR00003	74.75	0.005188			
4 VAR00004	15.78	0.006047			
5 VAR00005	59.74	0.002159			
6 VAR00006	55.89	0.014965			
7 VAR00007	85.96	0.008790			
8 VAR00008	70.46	0.006023			
10 VAR00010	24.83	0.002005			

Table S6. Classification matrix (cases in row categories classified into columns)

	BDA	HistA	PeDA	SperM	SpermD	TryptA	TyrA	%correct
BDA	83	1	0	0	0	0	0	99
HistA	0	72	0	0	0	12	0	86
PeDA	0	0	84	0	0	0	0	100
SperM	0	0	0	73	11	0	0	87
SpermD	0	0	4	18	62	0	0	74
TryptA	0	0	0	0	0	75	9	89
TyrA	0	0	0	0	0	3	81	96
Total	83	73	88	91	73	90	90	90

Table S7. Jackknifed classification matrix

	BDA	HistA	PeDA	SperM	SpermD	TryptA	TyrA	%correct
BDA	83	1	0	0	0	0	0	99
HistA	0	72	0	0	0	12	0	86
PeDA	0	0	84	0	0	0	0	100
SperM	0	0	0	71	13	0	0	85
SpermD	0	0	4	19	61	0	0	73
TryptA	0	0	0	0	0	74	10	88
TyrA	0	0	0	0	0	3	81	96
Total	83	73	88	90	74	89	91	89

Eigenvalues

Canonical correlations

0.987	0.872	0.809	0.682	0.485	0.178
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Cumulative proportion of total dispersion

0.860	0.930	0.973	0.992	0.999	1.000
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Wilks' lambda= 0.001
 Approx.F= 189.931 df= 48, 2828 p-tail= 0.0000

Pillai's trace= 3.121
 Approx.F= 78.465 df= 48, 3474 p-tail= 0.0000

Lawley-Hotelling trace= 44.627
 Approx.F= 532.114 df= 48, 3434 p-tail= 0.0000

Table S8. Canonical discriminant functions

	1	2	3	4	5	6
Constant	-210.738	165.427	472.014	-535.799	-727.664	-278.559
VAR00002	2570.259	2024.405	2053.760	1367.800	4010.962	2756.219
VAR00003	-2197.160	-5323.783	-12363.614	5885.433	7839.602	561.458
VAR00004	1542.382	3101.093	2787.986	1949.150	1620.206	2555.419
VAR00005	8121.792	-4939.713	-7419.670	5410.182	9667.847	3229.234
VAR00006	-7676.166	-991.531	-868.526	5470.299	3020.657	108.759
VAR00007	9697.833	2407.033	-5298.398	5191.521	6865.460	5157.672
VAR00008	-299.507	-8567.542	-5408.829	241.903	9163.249	-816.270
VAR00009
VAR00010	2316.137	528.331	-7277.546	13344.468	8686.948	7174.742

Table S9. Canonical discriminant functions -- standardized by within variances

	1	2	3	4	5	6
VAR00002	1.245	0.981	0.995	0.663	1.944	1.336
VAR00003	-1.613	-3.907	-9.074	4.319	5.754	0.412
VAR00004	1.794	3.607	3.243	2.267	1.884	2.972
VAR00005	8.709	-5.297	-7.956	5.802	10.367	3.463
VAR00006	-4.408	-0.569	-0.499	3.141	1.735	0.062
VAR00007	6.038	1.499	-3.299	3.232	4.274	3.211
VAR00008	-0.258	-7.383	-4.661	0.208	7.897	-0.703
VAR00009
VAR00010	1.968	0.449	-6.184	11.340	7.382	6.097

Table S10. Canonical scores of group means

	1	2	3	4	5	6
BDA	6.172	-0.249	1.484	-1.580	0.103	-0.166
HistA	4.975	-0.973	1.287	1.767	0.376	-0.043
PeDA	0.812	3.306	0.648	0.258	-0.712	0.128
SperM	-9.570	-2.423	0.979	-0.233	-0.412	0.135
SpermD	-9.240	1.682	-0.604	0.014	0.720	-0.174
TryptA	4.259	-0.281	-1.480	-0.460	0.587	0.308
TyrA	2.592	-1.061	-2.314	0.233	-0.662	-0.189

Analysis layer 1: Differentiate amines grouped by class

Table S11. Group frequencies

AliphAm	AromAm	PolyAm
168	252	168

Table S12. Group means

	AliphAm	AromAm	PolyAm
VAR00002	0.016	0.015	0.018
VAR00003	0.023	0.022	0.024
VAR00004	0.030	0.029	0.029
VAR00005	0.029	0.028	0.027
VAR00006	0.019	0.019	0.018
VAR00007	0.009	0.010	0.008
VAR00008	0.003	0.004	0.004
VAR00009	0.001	0.002	0.003
VAR00010	0.001	0.001	0.002

Table S13. Between groups F-matrix -- df = 8 578

	AliphAm	AromAm	PolyAm
AliphAm	0.000		
AromAm	104.225	0.000	
PolyAm	770.090	969.264	0.000

Wilks' lambda

Lambda = 0.0253 df = 8 2 585
 Approx. F= 381.6624 df = 16 1156 prob = 0.0000

Table S14. Classification functions

	AliphAm	AromAm	PolyAm
CONSTANT	-965454.691	-967871.452	-966080.336
VAR00002	5853548.909	5853263.132	5846121.255
VAR00003	2.23587E+07	2.24003E+07	2.23934E+07
VAR00004	7182676.994	7178859.161	7171172.385
VAR00005	2.25975E+07	2.26334E+07	2.25846E+07
VAR00006	1.12732E+07	1.12850E+07	1.13213E+07
VAR00007	1.77736E+07	1.77948E+07	1.77262E+07
VAR00008	1.58694E+07	1.58958E+07	1.59160E+07
VAR00009	0.000	0.000	0.000
VAR00010	3.49101E+07	3.49499E+07	3.49046E+07

Table S15.

Variable	F-to-remove	Tolerance	Variable	F-to-enter	Tolerance
2 VAR00002	5.69	0.074313	9 VAR00009	2.60	0.000827
3 VAR00003	180.40	0.003600			
4 VAR00004	6.23	0.005863			
5 VAR00005	116.63	0.002045			
6 VAR00006	75.54	0.013722			
7 VAR00007	133.39	0.010470			
8 VAR00008	145.89	0.005139			
10 VAR00010	61.77	0.001604			

Table S16. Classification matrix (cases in row categories classified into columns)

	AliphAm	AromAm	PolyAm	%correct
AliphAm	165	3	0	98
AromAm	2	250	0	99
PolyAm	0	5	163	97
Total	167	258	163	98

Table S17. Jackknifed classification matrix

	AliphAm	AromAm	PolyAm	%correct
AliphAm	162	6	0	96
AromAm	2	250	0	99
PolyAm	0	5	163	97
Total	164	261	163	98

Eigenvalues

15.279	1.425
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Canonical correlations

0.969	0.767
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Cumulative proportion of total dispersion

0.915	1.000
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Wilks' lambda= 0.025
 Approx.F= 381.662 df= 16, 1156 p-tail= 0.0000

Pillai's trace= 1.526
 Approx.F= 233.091 df= 16, 1158 p-tail= 0.0000

Lawley-Hotelling trace= 16.704
 Approx.F= 602.371 df= 16, 1154 p-tail= 0.0000

Table S18. Canonical discriminant functions

	1	2
Constant	-106.430	828.517
VAR00002	839.129	198.433
VAR00003	-965.926	-14608.354
VAR00004	1052.319	1452.751
VAR00005	4128.911	-12010.057
VAR00006	-4708.192	-4677.824
VAR00007	7045.146	-6557.040
VAR00008	-3457.603	-9605.694
VAR00009	.	.
VAR00010	3557.064	-13438.581

Table S19. Canonical discriminant functions -- standardized by within variances

	1	2
VAR00002	0.517	0.122
VAR00003	-0.888	-13.432
VAR00004	1.323	1.826
VAR00005	4.877	-14.187
VAR00006	-3.153	-3.133
VAR00007	4.565	-4.248
VAR00008	-3.453	-9.594
VAR00009	.	.
VAR00010	3.431	-12.962

Table S20. Canonical scores of group means

	1	2
AliphAm	2.261	1.751
AromAm	2.600	-1.122
PolyAm	-6.161	-0.068

Analysis layer 2: Differentiation within grouped amines - aliphatic amines

Table S21. Group frequencies

BDA	PeDA
84	84

Table S22. Group means

	BDA	PeDA
VAR00002	0.015	0.016
VAR00003	0.022	0.024
VAR00004	0.030	0.030
VAR00005	0.029	0.029
VAR00006	0.019	0.019
VAR00007	0.009	0.009
VAR00008	0.004	0.003
VAR00009	0.001	0.001
VAR00010	0.001	0.001

Table S23. Between groups F-matrix -- df = 9 158

	BDA	PeDA
BDA	0.000	
PeDA	1309.095	0.000

Wilks' lambda

Lambda = 0.0132 df = 9 1 166
 Approx. F= 1309.0951 df = 9 158 prob = 0.0000

Table S24. Classification functions

	BDA	PeDA
CONSTANT	-2780991.555	-2783074.142
VAR00002	2.98860E+07	2.99226E+07
VAR00003	4.32186E+07	4.32119E+07
VAR00004	4.44897E+07	4.46457E+07
VAR00005	4.66494E+07	4.65055E+07
VAR00006	3.55961E+07	3.57130E+07
VAR00007	5.92671E+07	5.92111E+07
VAR00008	3.23756E+07	3.21034E+07
VAR00009	2.96717E+07	2.98157E+07
VAR00010	7.07332E+07	7.08485E+07

Table S25.

Variable	F-to-remove	Tolerance	Variable	F-to-enter	Tolerance
2 VAR00002	1.70	0.059535			
3 VAR00003	0.03	0.096300			
4 VAR00004	17.41	0.027893			
5 VAR00005	11.14	0.018122			
6 VAR00006	8.23	0.017469			
7 VAR00007	1.05	0.118313			
8 VAR00008	46.05	0.040967			
9 VAR00009	8.08	0.037025			
10 VAR00010	4.45	0.034543			

Table S26. Classification matrix (cases in row categories classified into columns)

	BDA	PeDA	%correct
BDA	84	0	100
PeDA	0	84	100
Total	84	84	100

Table S27. Jackknifed classification matrix

	BDA	PeDA	%correct
BDA	84	0	100
PeDA	0	84	100
Total	84	84	100

Eigenvalues74.569Canonical correlations0.993Cumulative proportion of total dispersion1.000

Wilks' lambda= 0.013
 Approx.F= 1309.094 df= 9, 158 p-tail= 0.0000

Pillai's trace= 0.987
 Approx.F= 1309.094 df= 9, 158 p-tail= 0.0000

Lawley-Hotelling trace= 74.569
 Approx.F= 1309.095 df= 9, 158 p-tail= 0.0000

Table S28. Canonical discriminant functions

	1
Constant	-121.310
VAR00002	2131.928
VAR00003	-390.262
VAR00004	9083.775
VAR00005	-8387.702
VAR00006	6809.004
VAR00007	-3261.064
VAR00008	-15851.959
VAR00009	8393.316
VAR00010	6713.689

Table S29. Canonical discriminant functions -- standardized by within variances

	1
VAR00002	0.425
VAR00003	-0.044
VAR00004	1.899
VAR00005	-1.919
VAR00006	1.695
VAR00007	-0.238
VAR00008	-2.363
VAR00009	1.154
VAR00010	0.897

Table S30. Canonical scores of group means

	1
BDA	-8.584
PeDA	8.584

Analysis layer 2: Differentiation within grouped amines - aromatic amines

Table S31. Group frequencies

HistA	TryptA	TyrA
84	84	84

Table S32. Group means

	HistA	TryptA	TyrA
VAR00002	0.015	0.015	0.015
VAR00003	0.022	0.022	0.022
VAR00004	0.029	0.029	0.029
VAR00005	0.029	0.028	0.028
VAR00006	0.020	0.019	0.019
VAR00007	0.010	0.010	0.010
VAR00008	0.004	0.004	0.004
VAR00009	0.001	0.002	0.002
VAR00010	0.001	0.001	0.002

Table S33. Between groups F-matrix -- df = 9 241

	HistA	TryptA	TyrA
HistA	0.000		
TryptA	297.951	0.000	
TyrA	367.417	98.455	0.000

Wilks' lambda

Lambda = 0.0135 df = 9 2 249
 Approx. F= 203.8426 df = 18 482 prob = 0.0000

Table S34. Classification functions

	HistA	TryptA	TyrA
CONSTANT	-2140604.318	-2139166.569	-2138362.364
VAR00002	1.67778E+07	1.67939E+07	1.67523E+07
VAR00003	3.09272E+07	3.09238E+07	3.09461E+07
VAR00004	3.76131E+07	3.75863E+07	3.75813E+07
VAR00005	3.63952E+07	3.63874E+07	3.63876E+07
VAR00006	3.11592E+07	3.11098E+07	3.11033E+07
VAR00007	3.92106E+07	3.92562E+07	3.92167E+07
VAR00008	2.45970E+07	2.45822E+07	2.45512E+07
VAR00009	4.60522E+07	4.59953E+07	4.60748E+07
VAR00010	4.12095E+07	4.12601E+07	4.12239E+07

Table S35.

Variable	F-to-remove	Tolerance	Variable	F-to-enter	Tolerance
2 VAR00002	86.85	0.096924			
3 VAR00003	4.40	0.018273			
4 VAR00004	2.33	0.013660			
5 VAR00005	0.19	0.049563			
6 VAR00006	8.52	0.040055			
7 VAR00007	11.25	0.049903			
8 VAR00008	5.81	0.057055			
9 VAR00009	12.34	0.010695			
10 VAR00010	5.11	0.018330			

Table S36. Classification matrix (cases in row categories classified into columns)

	HistA	TryptA	TyrA	%correct
HistA	84	0	0	100
TryptA	0	82	2	98
TyrA	0	0	84	100
Total	84	82	86	99

Table S37. Jackknifed classification matrix

	HistA	TryptA	TyrA	%correct
HistA	84	0	0	100
TryptA	0	82	2	98
TyrA	0	1	83	99
Total	84	83	85	99

Eigenvalues

15.529	3.487
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Canonical correlations

0.969	0.882
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Cumulative proportion of total dispersion

0.817	1.000
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Wilks' lambda= 0.013
 Approx.F= 203.843 df= 18, 482 p-tail= 0.0000

Pillai's trace= 1.717
 Approx.F= 162.909 df= 18, 484 p-tail= 0.0000

Lawley-Hotelling trace= 19.016
 Approx.F= 253.551 df= 18, 480 p-tail= 0.0000

Table S38. Canonical discriminant functions

	1	2
Constant	-229.178	-117.725
VAR00002	1103.715	8927.779
VAR00003	-1223.478	-4603.832
VAR00004	3567.367	167.490
VAR00005	915.357	-300.405
VAR00006	6371.152	-263.593
VAR00007	-2566.802	9433.556
VAR00008	4022.058	5778.866
VAR00009	1004.875	-17903.536
VAR00010	-3410.357	8943.024

Table S39. Canonical discriminant functions -- standardized by within variances

	1	2
VAR00002	0.289	2.337
VAR00003	-0.402	-1.512
VAR00004	1.216	0.057
VAR00005	0.176	-0.058
VAR00006	1.324	-0.055
VAR00007	-0.387	1.421
VAR00008	0.563	0.809
VAR00009	0.187	-3.336
VAR00010	-0.594	1.558

Table S40. Canonical scores of group means

	1	2
HistA	5.496	-0.329
TryptA	-2.147	2.420
TyrA	-3.349	-2.091

Analysis layer 2: Differentiation within grouped amines - polyamines

Table S41. Group frequencies

SperM	SpermD
84	84

Table S42. Group means

	SperM	SpermD
VAR00002	0.018	0.018
VAR00003	0.023	0.025
VAR00004	0.028	0.029
VAR00005	0.027	0.028
VAR00006	0.018	0.018
VAR00007	0.008	0.008
VAR00008	0.004	0.003
VAR00009	0.004	0.002
VAR00010	0.003	0.002

Table S43. Between groups F-matrix -- df = 7 160

	SperM	SpermD
SperM	0.000	
SpermD	60.668	0.000

Wilks' lambda

Lambda = 0.2737 df = 7 1 166
 Approx. F= 60.6683 df = 7 160 prob = 0.0000

Table S44. Classification functions

	SperM	SpermD
CONSTANT	-81126.458	-81605.233
VAR00002	-528014.263	-528452.629
VAR00003	4270034.920	4282858.067
VAR00004	-1570378.045	-1572802.104
VAR00005	4353261.332	4366115.964
VAR00006	-2175684.026	-2190480.089
VAR00007	2624955.188	2643826.671
VAR00008	4159658.295	4164993.503
VAR00009	0.000	0.000
VAR00010	0.000	0.000

Table S45.

Variable	F-to-remove	Tolerance	Variable	F-to-enter	Tolerance
2 VAR00002	0.12	0.080826	9 VAR00009	4.91	0.000283
3 VAR00003	11.52	0.003448	10 VAR00010	0.26	0.000688
4 VAR00004	1.44	0.004844			
5 VAR00005	12.95	0.001670			
6 VAR00006	27.76	0.009492			
7 VAR00007	50.04	0.007335			
8 VAR00008	2.64	0.003236			

Table S46. Classification matrix (cases in row categories classified into columns)

	SperM	SperMD	%correct
SperM	82	2	98
SperMD	11	73	87
Total	93	75	92

Table S47. Jackknifed classification matrix

	SperM	SperMD	%correct
SperM	81	3	96
SperMD	15	69	82
Total	96	72	89

Eigenvalues2.654Canonical correlations0.852Cumulative proportion of total dispersion1.000

Wilks' lambda= 0.274
 Approx.F= 60.668 df= 7, 160 p-tail= 0.0000

Pillai's trace= 0.726
 Approx.F= 60.668 df= 7, 160 p-tail= 0.0000

Lawley-Hotelling trace= 2.654
 Approx.F= 60.668 df= 7, 160 p-tail= 0.0000

Table S48. Canonical discriminant functions

	1
Constant	147.820
VAR00002	135.343
VAR00003	-3959.088
VAR00004	748.417
VAR00005	-3968.809
VAR00006	4568.217
VAR00007	-5826.484
VAR00008	-1647.221
VAR00009	.
VAR00010	.

Table S49. Canonical discriminant functions -- standardized by within variances

	1
VAR00002	0.112
VAR00003	-5.178
VAR00004	1.591
VAR00005	-7.855
VAR00006	4.630
VAR00007	-6.687
VAR00008	-2.629
VAR00009	.
VAR00010	.

Table S50. Canonical scores of group means

	1
SperM	1.619
SpermD	-1.619

Analysis Layer 3: Determination of analyte concentration - Histamine

Principal Components

Variable	Components								
	1	2	3	4	5	6	7	8	9
Var2	-0.0996517	0.19603688	0.59420967	-0.49225298	0.49363214	-0.03725154	0.2972222	0.10087007	0.11253757
Var3	-0.5848758	0.18277998	0.08939255	-0.26868102	-0.48536	0.09730824	-0.31787822	0.09066675	0.43591383
Var4	-0.6068441	-0.2121961	-0.1283041	0.4371433	0.16082656	-0.06002935	0.56579781	0.03871043	0.16751797
Var5	0.1190467	-0.6428119	0.29395112	0.20383555	0.25526008	0.13747677	-0.39851001	0.1241919	0.43170947
Var6	0.30444878	-0.4353842	-0.0654417	-0.39148328	-0.46100751	0.10407004	0.52899736	0.15724172	0.17968868
Var7	0.04330348	-0.0073835	-0.6306344	-0.35224214	0.36686978	-0.38719746	-0.09097931	-0.08546247	0.41976118
Var8	0.0907756	0.27757123	-0.3157123	0.03848746	0.23055997	0.72018254	0.04240509	0.47438017	0.12207749
Var9	0.29712394	0.32790411	0.12508006	0.25374618	-0.07220192	0.19103236	0.19675352	-0.59662783	0.53645211
Var10	0.27289292	0.30942827	0.13694037	0.33113772	-0.15568422	-0.50073075	0.05522116	0.59300297	0.26778334

Variance	0.00000058	0.00000014	0.00000001	0	0	0	0	0	0
Variance%	78.5836257	19.0674610	1.46593022	0.54443502	0.12675329	0.09929826	0.06973325	0.02637853	0.01638013
Cum%	78.5836257	97.6510925	99.1170196	99.6614532	99.7882080	99.8875045	99.9572372	99.9836196	100
P-value									

Standardized Principal Components

Variable	Components								
	1	2	3	4	5	6	7	8	9
Var2	-130.618896	521.6490479	5702.563965	-7751.79736	16110.56934	-1373.60071	13078.21191	7216.458496	10217.05957
Var3	-766.628113	486.3728027	857.8903198	-4231.07813	-15840.5938	3588.111084	-13987.1074	6486.491699	39575.73828
Var4	-795.423157	-564.648376	-1231.32056	6883.952637	5248.863281	-2213.50195	24895.93359	2769.42627	15208.62012
Var5	156.0409393	-1710.50598	2821.016113	3209.918213	8330.870117	5069.271973	-17535.0254	8884.951172	39194.03516
Var6	399.057312	-1158.54626	-628.03717	-6164.91748	-15045.8066	3837.443115	23276.66016	11249.40625	16313.57324
Var7	56.76018906	-19.6475105	-6052.12793	-5546.96436	11973.45313	-14277.3877	-4003.2229	-6114.1665	38109.27344
Var8	118.9844437	738.6098633	-3029.85596	606.0846558	7524.737793	26555.76563	1865.885986	33938.16406	11083.16992
Var9	389.4562683	872.5443115	1200.379395	3995.890381	-2356.43896	7044.0625	8657.443359	-42684.0195	48703.40625
Var10	357.6953735	823.3806152	1314.201416	5214.620605	-5081.03369	-18463.7754	2429.811768	42424.69141	24311.51172

Variance	0.00000058	0.00000014	0.00000001	0	0	0	0	0	0
Variance%	78.58362579	19.06746101	1.46593022	0.54443502	0.12675329	0.09929826	0.06973325	0.02637853	0.01638013
Cum%	78.58362579	97.65109253	99.11701965	99.66145325	99.78820801	99.88750458	99.95723724	99.98361969	100
P-value									

References for the supporting information

- (1) E. M. Enlow, J. L. Kennedy, A. A. Nieuwland, J. E. Hendrix, S. L. Morgan *Appl. Spectrosc.* **2005**, *59*, 986-992.