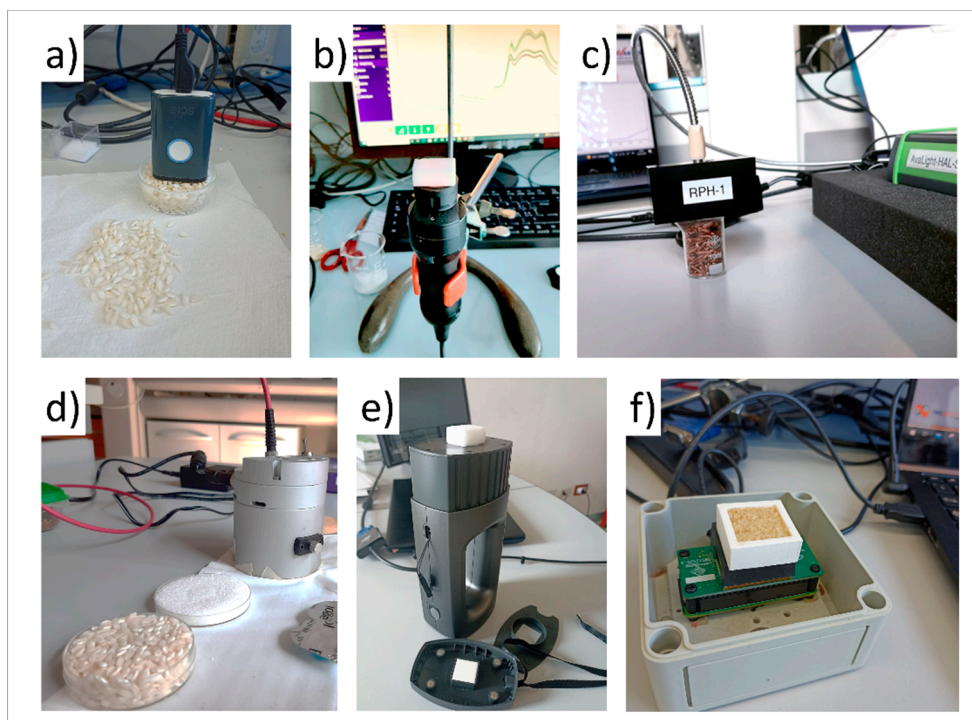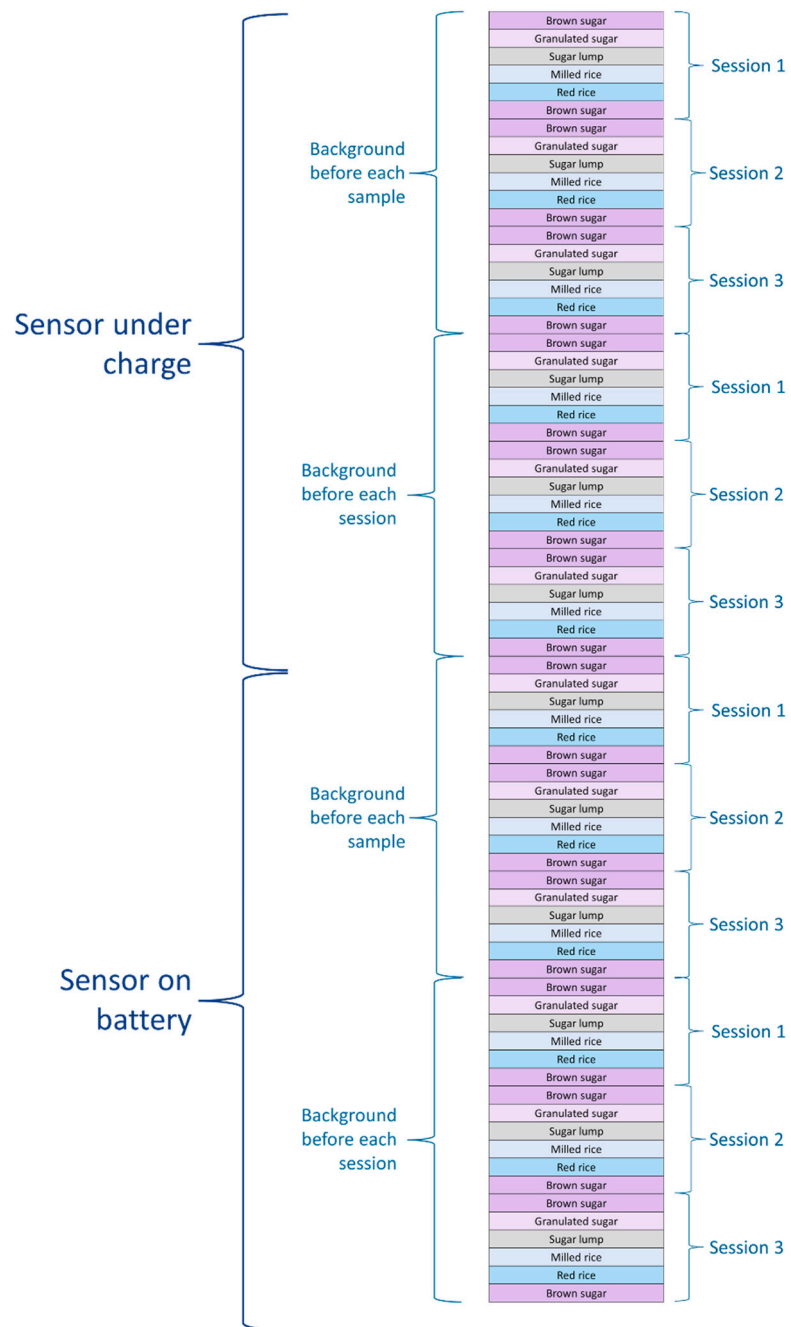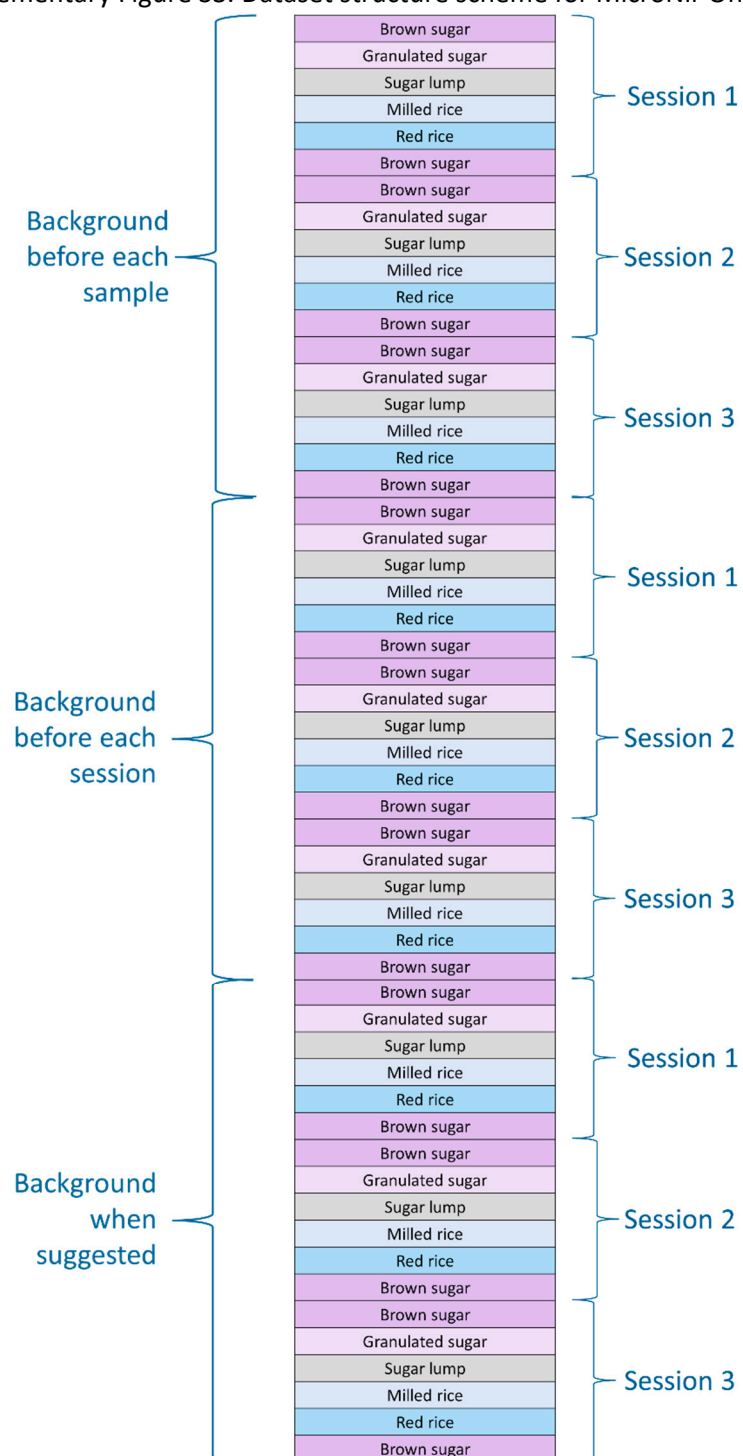# Supplementary materials

Supplementary Figure S1. Examples of spectrometer positioning during the analyses: (a) SCiO, (b) Viavi Micro-NIR, (c) AvaSpec with optical fibre, (d) AvaSpec with integrating sphere, (e) NeoSpectra Scanner, (f) NeoSpectra Development kit
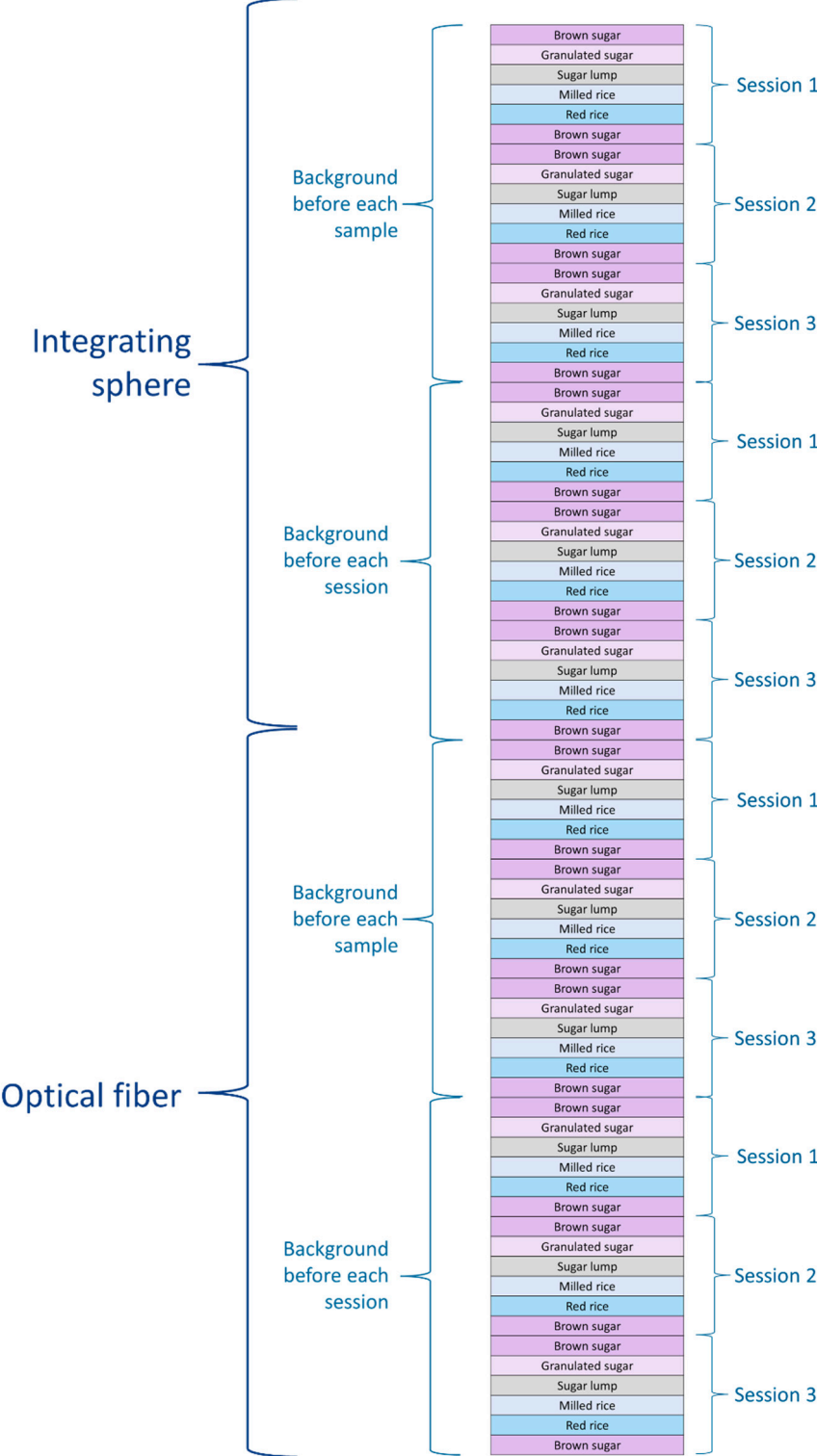
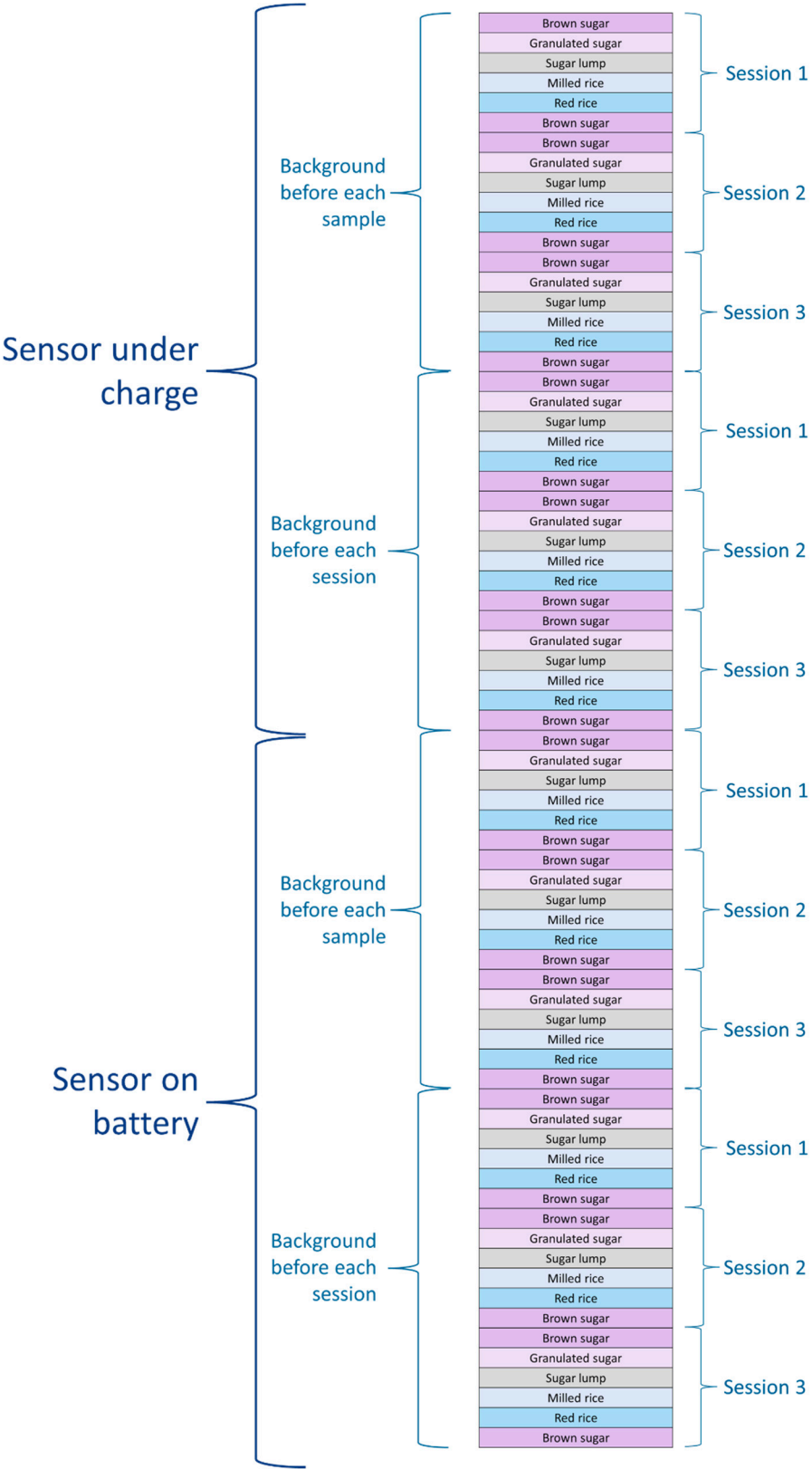# Supplementary Figure S2. Dataset structure scheme for SCiO

Supplementary Figure S3. Dataset structure scheme for MicroNir OnSite-W

Background before each sample

Session 1
- Brown sugar
- Granulated sugar
- Sugar lump
- Milled rice
- Red rice
- Brown sugar

Session 2
- Brown sugar
- Granulated sugar
- Sugar lump
- Milled rice
- Red rice
- Brown sugar

Session 3
- Brown sugar
- Granulated sugar
- Sugar lump
- Milled rice
- Red rice
- Brown sugar

Background before each session

Session 1
- Brown sugar
- Granulated sugar
- Sugar lump
- Milled rice
- Red rice
- Brown sugar

Session 2
- Brown sugar
- Granulated sugar
- Sugar lump
- Milled rice
- Red rice
- Brown sugar

Session 3
- Brown sugar
- Granulated sugar
- Sugar lump
- Milled rice
- Red rice
- Brown sugar

Background when suggested

Session 1
- Brown sugar
- Granulated sugar
- Sugar lump
- Milled rice
- Red rice
- Brown sugar

Session 2
- Brown sugar
- Granulated sugar
- Sugar lump
- Milled rice
- Red rice
- Brown sugar

Session 3
- Brown sugar
- Granulated sugar
- Sugar lump
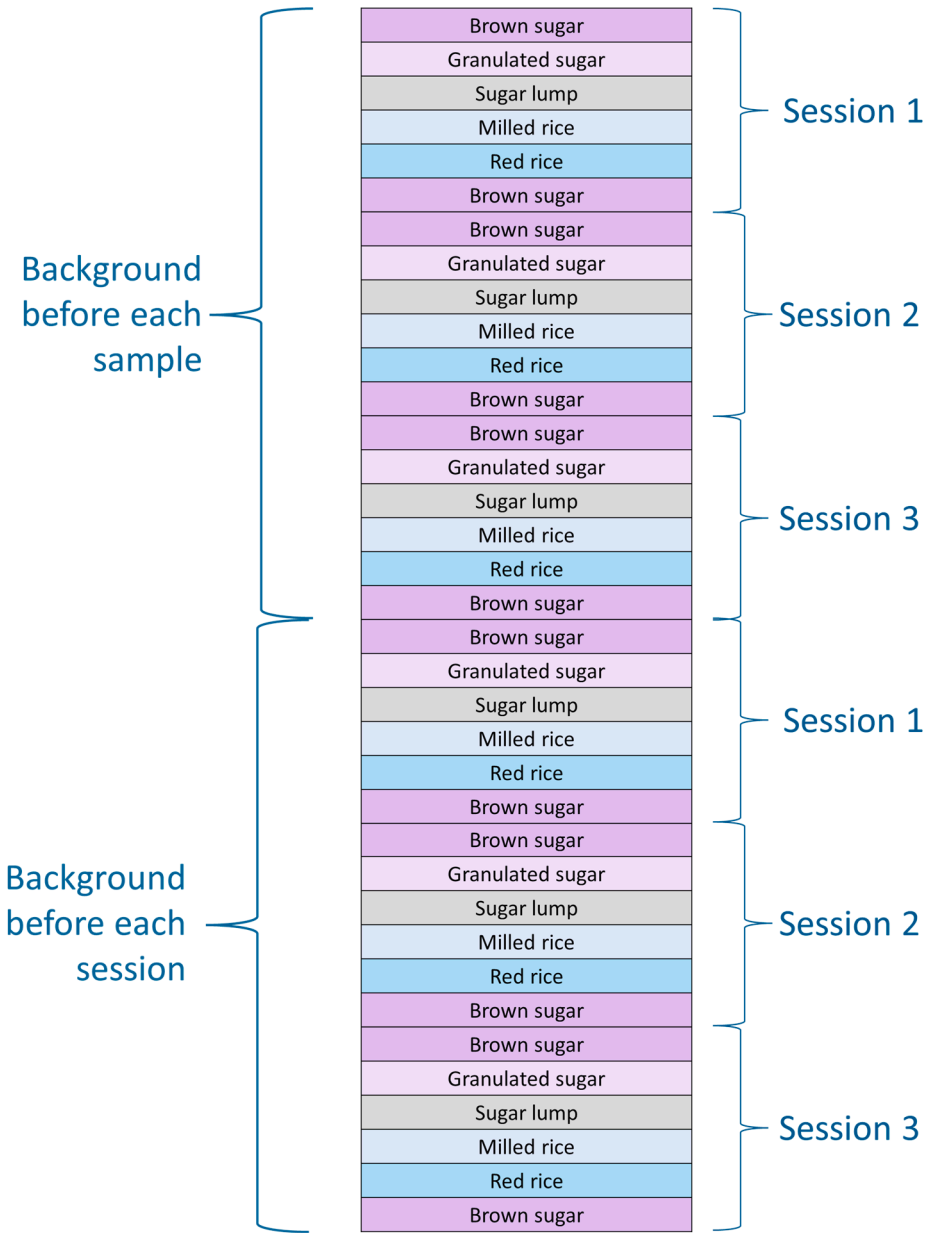- Milled rice
- Red rice
- Brown sugar

Supplementary Figure S4. Dataset structure scheme for AvaSpec-Mini NIR

Supplementary Figure S5. Dataset structure scheme for NeoSpectra Scanner

Supplementary Figure S6. Dataset structure scheme for NeoSpectra development kit

Background before each sample

Background before each session

|	
Brown sugar	
Granulated sugar	
Sugar lump	Session 1
Milled rice	
Red rice	
Brown sugar	
Brown sugar	
Granulated sugar	
Sugar lump	Session 2
Milled rice	
Red rice	
Brown sugar	
Brown sugar	
Granulated sugar	
Sugar lump	Session 3
Milled rice	
Red rice	
Brown sugar	
Brown sugar	
Granulated sugar	
Sugar lump	Session 1
Milled rice	
Red rice	
Brown sugar	
Brown sugar	
Granulated sugar	
Sugar lump	Session 2
Milled rice	
Red rice	
Brown sugar	
Brown sugar	
Granulated sugar	
Sugar lump	Session 3
Milled rice	
Red rice	
Brown sugar	

Supplementary Figure S7. Averaged spectra of each sample with the different spectrometers: (a) SCiO, (b) Viavi Micro-NIR, (c) AvaSpec with integrating sphere, (d) AvaSpec with optical fiber, (e) NeoSpectra Scanner, (f) NeoSpectra Development kit
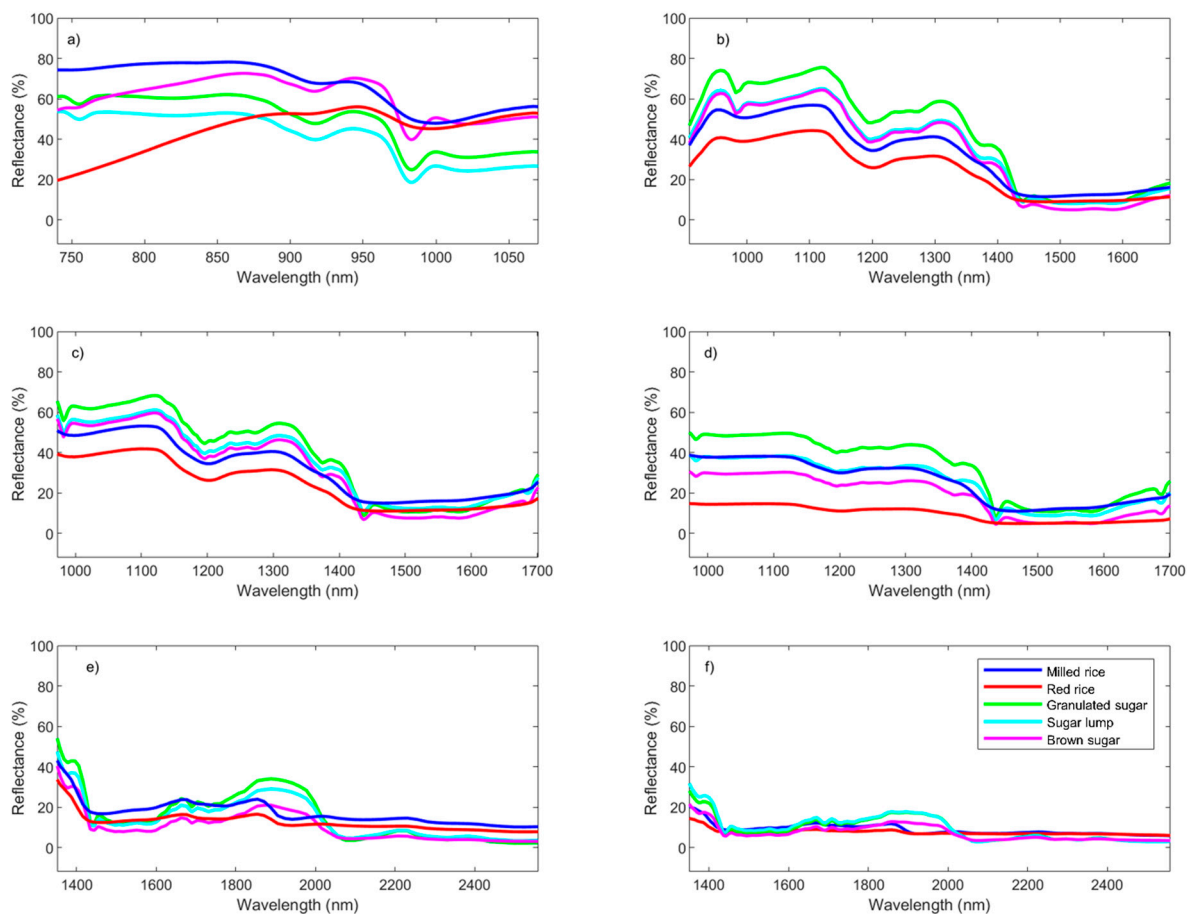
Supplementary Figure S8. PCA results on data preprocessed with MSC: Score plot for (a) SCiO, (b) Viavi Micro-NIR, (c) AvaSpec with integrating sphere, (d) AvaSpec with optical fibre, (e) NeoSpectra Scanner, (f) NeoSpectra Development kit.
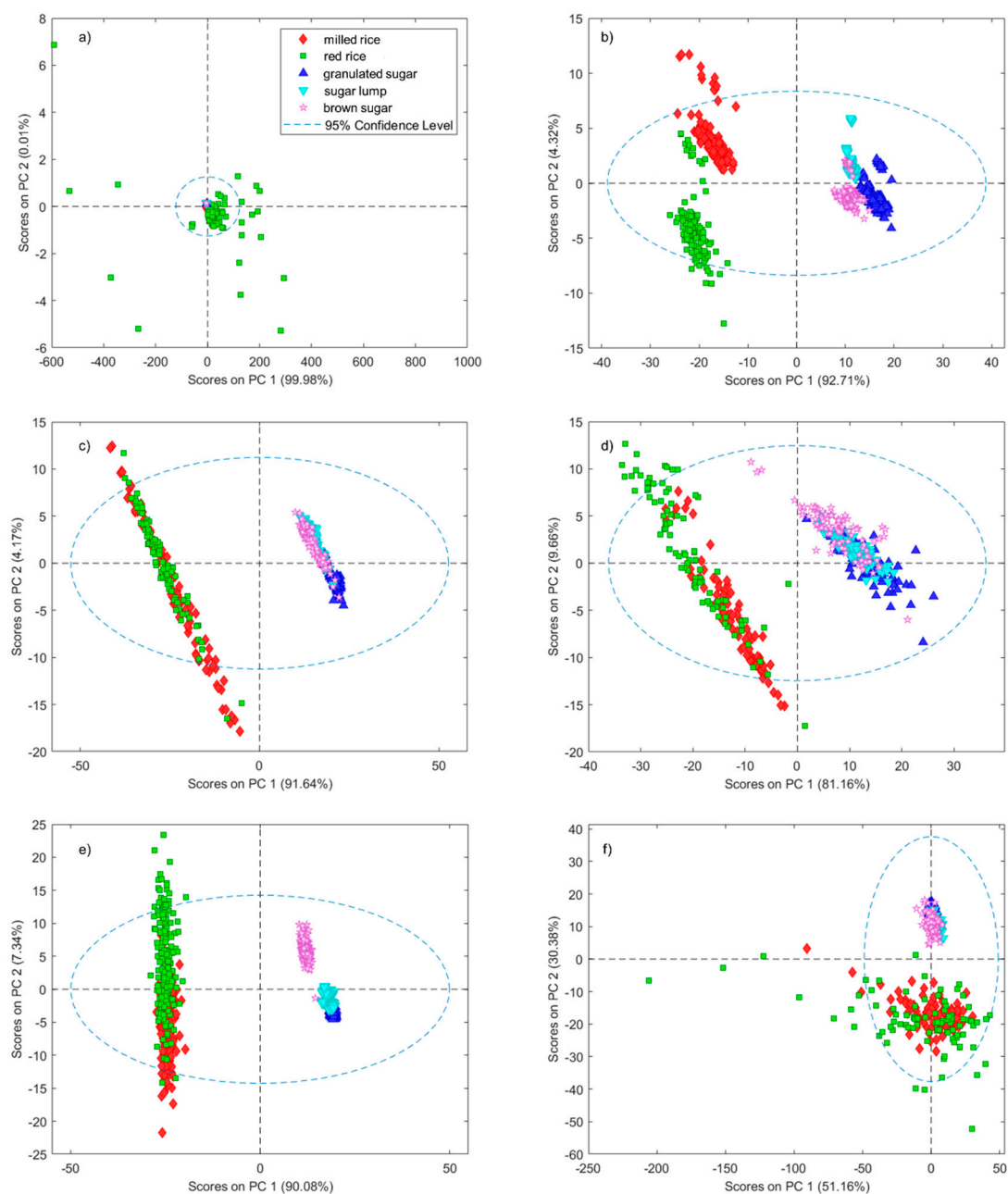
Supplementary Figure S9. PCA results on data preprocessed with MSC: Loading plot for (a) SCiO, (b) Viavi Micro-NIR, (c) AvaSpec with integrating sphere, (d) AvaSpec with optical fiber, (e) NeoSpectra Scanner, (f) NeoSpectra Development kit.
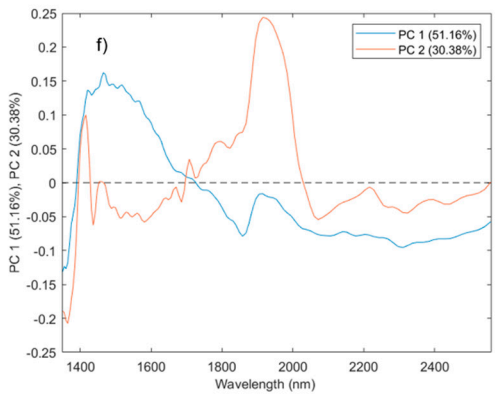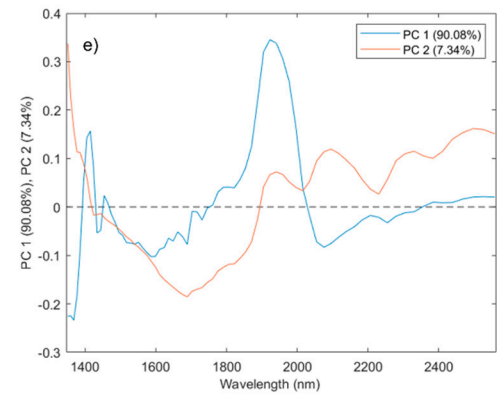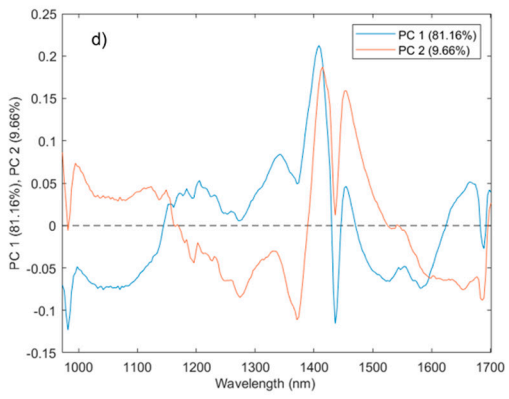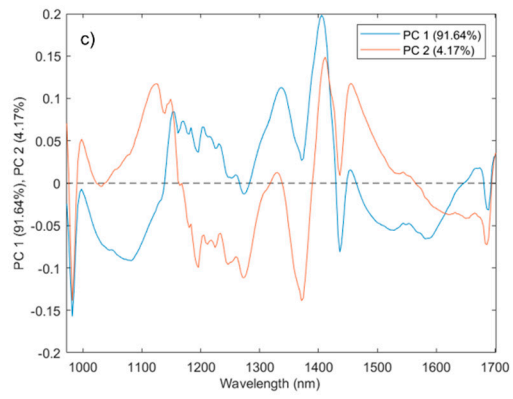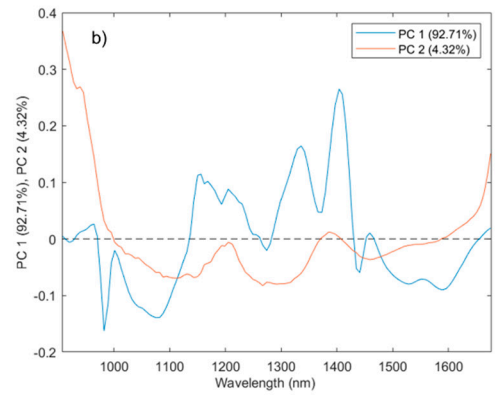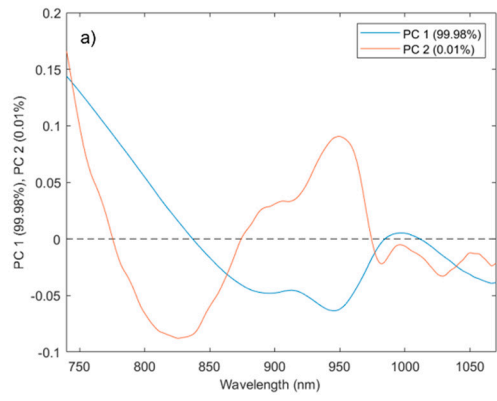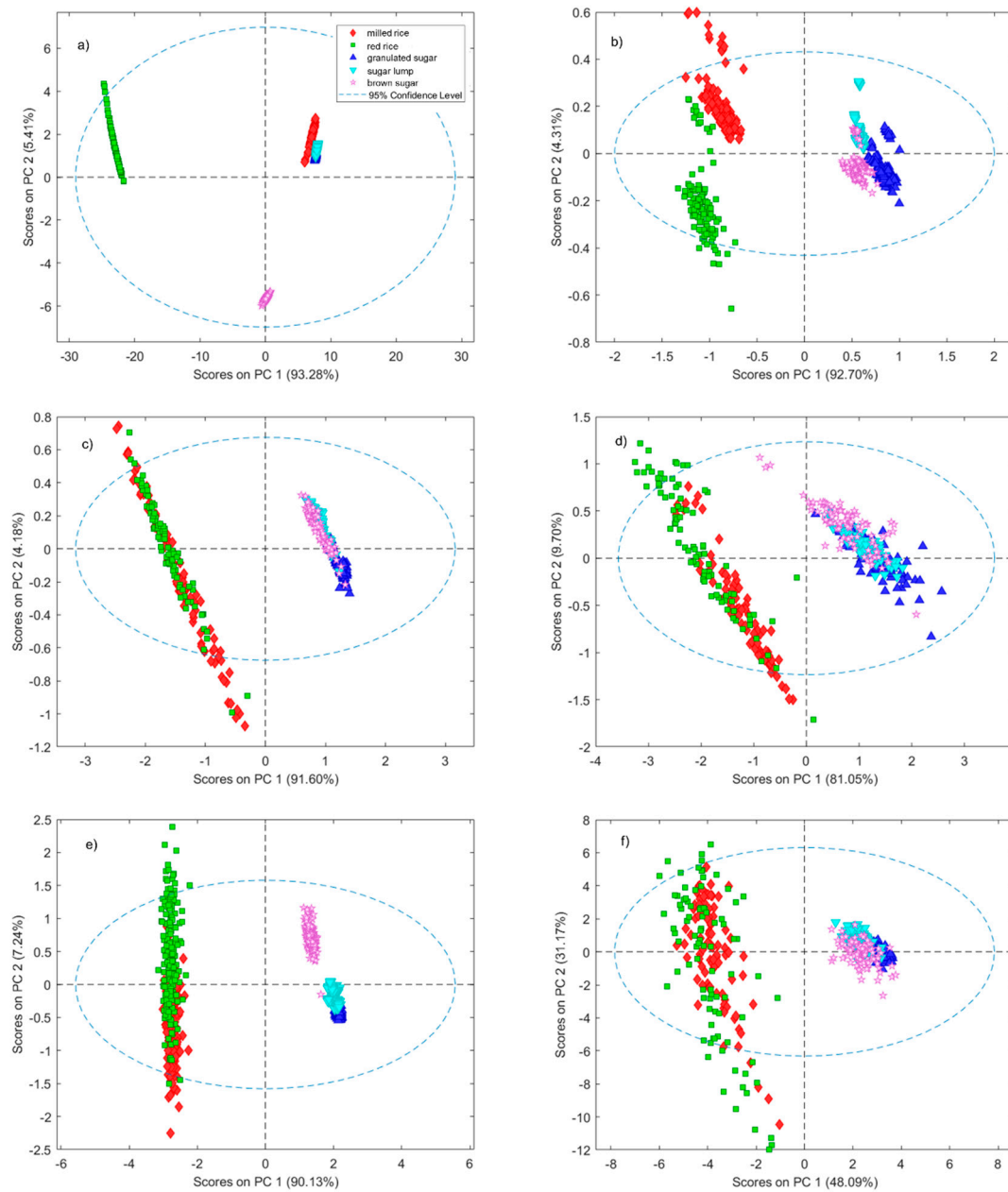
Supplementary Figure S10. PCA results on data preprocessed with SNV: Score plot for (a) SCiO, (b) Viavi Micro-NIR, (c) AvaSpec with integrating sphere, (d) AvaSpec with optical fibre, (e) NeoSpectra Scanner, (f) NeoSpectra Development kit.

Supplementary Figure S11. PCA results on data preprocessed with SNV: Loading plot for (a) SCiO, (b) Viavi Micro-NIR, (c) AvaSpec with integrating sphere, (d) AvaSpec with optical fiber, (e) NeoSpectra Scanner, (f) NeoSpectra Development kit.
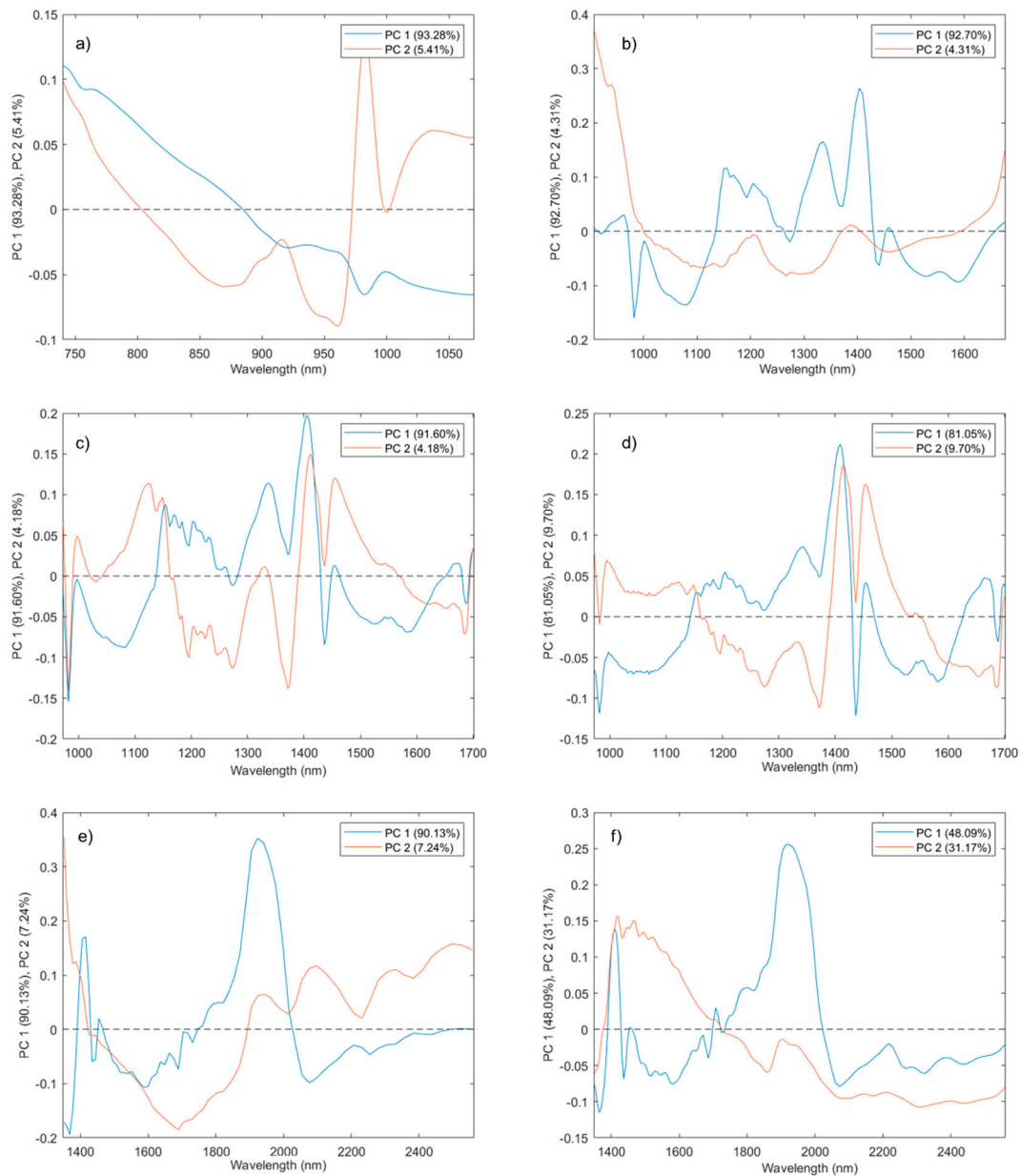
Supplementary Table S1. Resume of results for ASCA models of SCiO data. Effect in percentage which represent the contribution to the sum of squares of the data and cumulative eigenvalue. Models calculated on each type of sample according to the macro-chemical characteristics. In bold are reported factors that shown a p-value < 0.05 after 200 permutations. The factor "sample" included as sample levels respectively milled rice, brown rice, granulated sugar, sugar lump and only the replicate of the brown sugar acquired at the beginning of each session.

Factors	Effects		
	Samples (all)	Rice samples	Sugar samples
Sample	**74.95**	**71.22**	**72.43**
Order of replicates	0.49	1.28	**1.84**
Session	0.12	0.22	0.10
Power supply	0.00	0.01	0.01
Timing of background	**0.30**	**0.35**	**0.39**
Sample x Order of replicates	**2.53**	1.45	**2.87**
Sample x Session	0.16	0.14	0.16
Sample x Power supply	0.13	0.18	0.06

Sample x Timing of background	**0.37**	**0.57**	0.09
Order of replicates x Session	0.51	2.07	0.62
Order of replicates x Power supply	**0.85**	1.54	**1.54**
Order of replicates x Timing of background	0.19	0.56	0.44
Session x Power supply	0.10	0.25	0.04
Session x Timing of background	0.05	0.23	0.01
Power supply x Timing of background	0.04	0.11	0.01
Residuals	19.20	19.83	19.39

Supplementary Table S2. Resume of results for ASCA models of MicroNIR data. Effect in percentage which represent the contribution to the sum of squares of the data and cumulative eigenvalue. Models calculated on each type of sample according to the macro-chemical characteristics. In bold are reported factors that shown a p-value < 0.05 after 200 permutations. The factor "sample" included as sample levels respectively milled rice, brown rice, granulated sugar, sugar lump and only the replicate of the brown sugar acquired at the beginning of each session.

Factors	Effects		
	Samples (all)	Rice samples	Sugar samples
Sample	**90.89**	**76.65**	**81.02**
Order of replicates	0.14	**1.74**	0.35
Session	**0.65**	**1.33**	**2.04**
Timing of background	**0.70**	**1.03**	**2.11**
Sample x Order of replicates	**0.73**	**1.73**	0.38
Sample x Session	**0.25**	0.63	1.37
Sample x Timing of background	**1.98**	0.38	7.30
Order of replicates x Session	0.10	1.45	0.04
Order of replicates x Timing of background	0.12	1.96	0.04
Session x Timing of background	**0.39**	**2.11**	**1.18**
Residuals	4.05	10.98	4.16

Supplementary Table S3. Resume of results for ASCA models of AvaSpec-mini-NIR data. Effect in percentage which represent the contribution to the sum of squares of the data and cumulative eigenvalue. Models calculated on each type of sample according to the macro-chemical characteristics. In bold are reported factors that shown a p-value < 0.05 after 200 permutations. The factor "sample" included as sample levels respectively milled rice, brown rice, granulated sugar, sugar lump and only the replicate of the brown sugar acquired at the beginning of each session.

Factors	Effects					
	Optical fiber			Integrating sphere		
	Samples (all)	Rice samples	Sugar samples	Samples (all)	Rice samples	Sugar samples
Sample	**33.83**	**43.30**	**18.25**	**64.46**	**28.49**	**60.48**
Number of replicates	2.21	3.84	3.48	1.08	5.83	0.97
Session	0.55	1.58	0.73	0.21	0.14	**1.22**
Timing of background	**0.86**	**2.24**	0.55	0.24	0.43	**0.68**
Sample x Number of replicates	8.82	4.21	10.48	3.44	4.09	1.92
Sample x Session	**3.21**	0.88	**3.97**	**1.12**	1.03	**4.25**
Sample x Timing of background	**1.40**	0.18	**1.96**	**1.26**	0.70	**5.93**

Number of replicates x Session	2.50	8.68	6.68	2.34	12.38	2.16
Number of replicates x Timing of background	1.61	3.53	3.57	0.89	6.14	0.56
Session x Timing of background	**0.77**	0.78	0.94	0.09	0.56	**1.25**
Residuals	44.24	30.77	49.39	24.87	40.21	20.58

Supplementary Table S4. Resume of results for ASCA models of NeoSpectra Scanner data. Effect in percentage which represent the contribution to the sum of squares of the data and cumulative eigenvalue. Models calculated on each type of sample according to the macro-chemical characteristics. In bold are reported factors that shown a p-value < 0.05 after 200 permutations. The factor "sample" included as sample levels respectively milled rice, brown rice, granulated sugar, sugar lump and only the replicate of the brown sugar acquired at the beginning of each session.

Factors	Effects		
	Samples (all)	Rice samples	Sugar samples
Sample	**90.24**	**58.24**	**94.53**
Order of replicates	0.10	1.21	0.06
Session	**0.04**	0.54	**0.11**
Power supply	**0.04**	0.02	**0.17**
Timing of background	0.01	0.04	**0.05**
Sample x Order of replicates	0.39	1.08	0.12
Sample x Session	**0.29**	0.42	**0.42**
Sample x Power supply	**0.16**	**0.54**	0.15
Sample x Timing of background	**0.16**	0.28	**0.35**
Order of replicates x Session	0.20	2.62	0.10
Order of replicates x Power supply	0.15	2.24	0.03
Order of replicates x Timing of background	0.13	1.79	0.06
Session x Power supply	0.02	0.14	**0.12**
Session x Timing of background	**0.05**	0.04	**0.17**
Power supply x Timing of background	0.03	0.22	**0.11**
Residuals	8.00	30.58	3.45

Supplementary Table S5. Resume of results for ASCA models of NeoSpectra development kit data. Effect in percentage which represent the contribution to the sum of squares of the data and cumulative eigenvalue. Models calculated on each type of sample according to the macro-chemical characteristics. In bold are reported factors that shown a p-value < 0.05 after 200 permutations. The factor "sample" included as sample levels respectively milled rice, brown rice, granulated sugar, sugar lump and only the replicate of the brown sugar acquired at the beginning of each session.

Factors	Effects		
	Samples (all)	Rice samples	Sugar samples
Sample	**51.73**	**9.87**	**55.00**
Order of replicates	1.52	8.19	1.13
Session	0.03	0.21	0.20
Timing of background	0.22	0.05	**1.03**
Sample x Order of replicates	**7.27**	9.87	4.47
Sample x Session	**2.55**	2.40	**5.70**
Sample x Timing of background	**1.54**	0.73	**4.53**

Order of replicates x Session	2.62	10.19	3.74
Order of replicates x Timing of background	**2.53**	**11.79**	2.53
Session x Time of background	0.44	1.16	**0.77**
Residuals	29.56	45.54	20.89