Electronic Supplementary Material (ESI) for Analyst.

Electronic Supplementary Information

Determination of meningioma brain tumour grades using Raman microspectroscopy imaging

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Table S1: Correct classification rate for distinguishing Grade I and Grade II meningiomas.

Algorithm	**Class**	**Training**	**Test**
PCA-LDA	Grade I	80.0	31.6
	Grade II	66.7	85.7
PCA-QDA	Grade I	97.8	100
	Grade II	73.3	85.7
PCA-SVM	Grade I	100	73.7
	Grade II	100	28.6
SPA-LDA	Grade I	75.6	42.1
	Grade II	66.7	100
SPA-QDA	Grade I	95.6	100
	Grade II	46.7	85.7
SPA-SVM	Grade I	77.8	21.1
	Grade II	100	71.4
GA-LDA	Grade I	100	63.2
	Grade II	93.3	57.1
GA-QDA	Grade I	100	100
	Grade II	86.7	0
GA-SVM	Grade I	91.1	42.1
	Grade II	100	42.9

Figure S1: Outliers identified by a Hotelling T^2 *versus* Q residuals test (PCA with 8 PCs). (a) Meningioma Grade I samples (outliers: 58, 66); (b) meningioma Grade II samples (outliers: 11, 18); (c) meningioma Grade I outlier spectra in red; (d) meningioma Grade II outlier spectra in red.

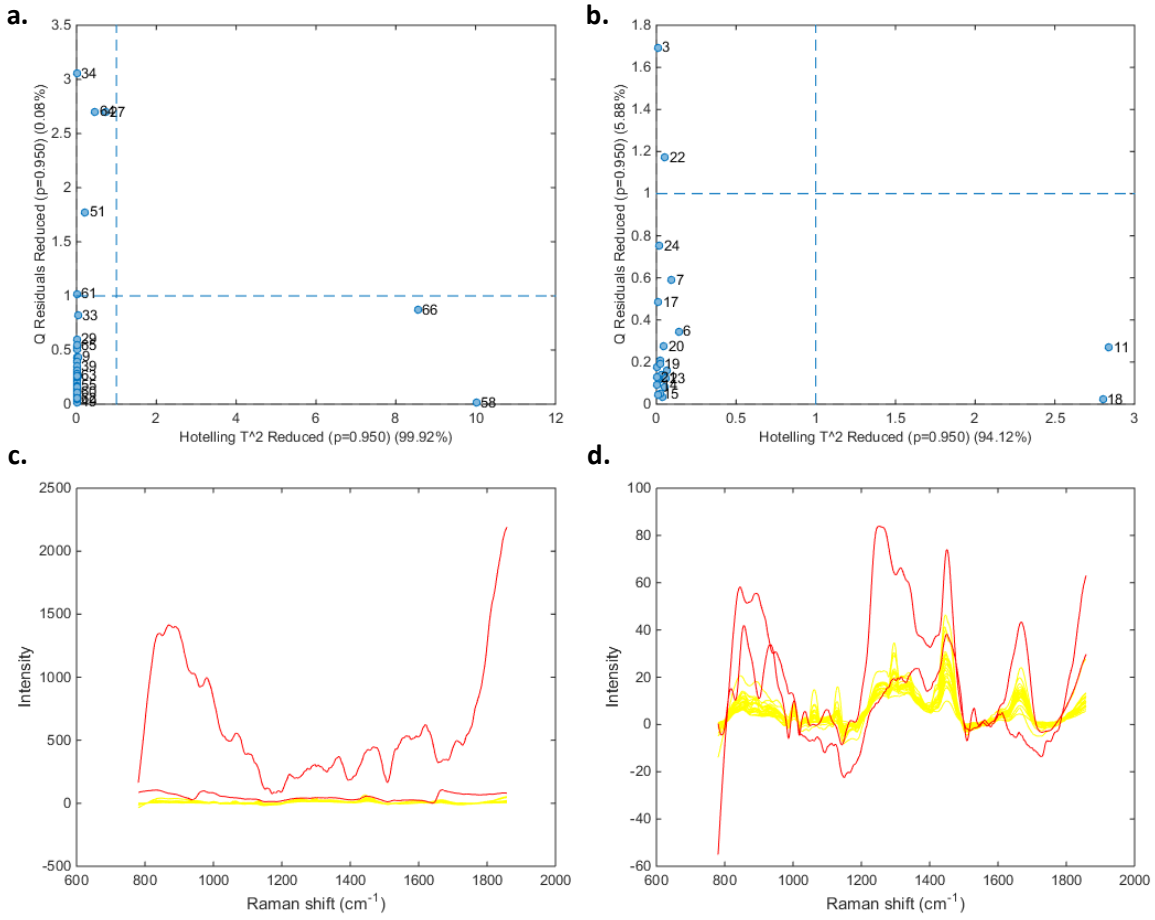

Figure S2: Singular value varying the number of principal components (PCs) of PCA.

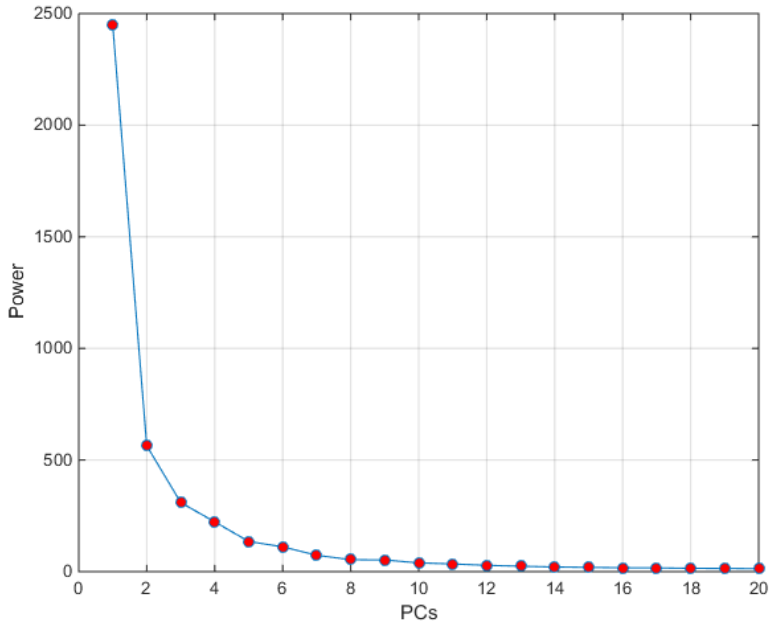

Figure S3: Concentration distribution maps and recovered spectral profiles by MCR-ALS for the 1st (a), 2nd (b), 3rd (c), and 4th (d) components. Colour bar: relative concentration.