## **Supplementary Information**

## Spectral classification for diagnosis involving numerous pathologies in a complex clinical setting: a neuro-oncology example

Danielle Bury<sup>a</sup>, Camilo L M Morais<sup>a</sup>, Maria Paraskevaidi<sup>a</sup>, Katherine M Ashton<sup>b</sup>, Timothy P Dawson<sup>b</sup>, Francis L Martin<sup>a</sup>

<sup>a</sup>School of Pharmacy and Biomedical Sciences, University of Central Lancashire, Preston PR1 2HE, UK

**Corresponding Author:** Professor Francis L Martin, School of Pharmacy and Biomedical Sciences, University of Central Lancashire, Preston PR1 2HE, UK; Tel.: +44(0)1772 896482; Email: flmartin@uclan.ac.uk

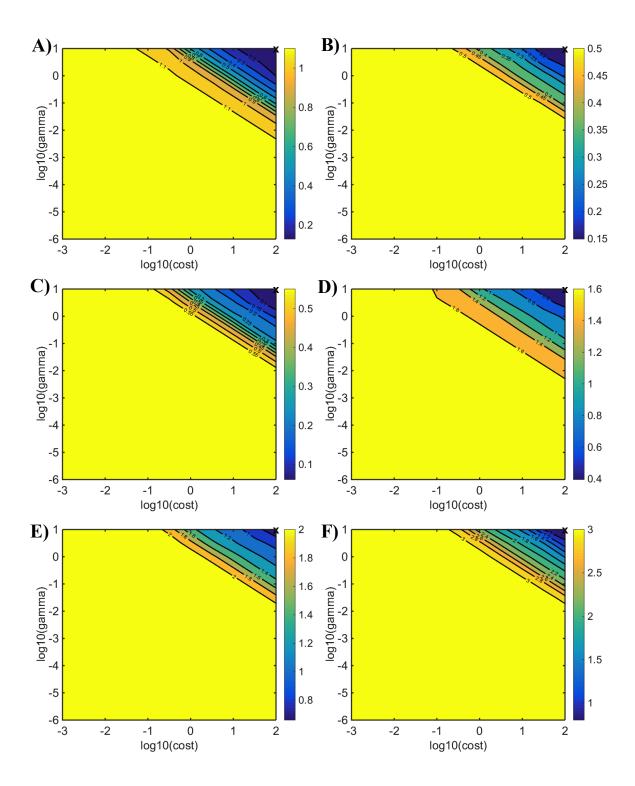
<sup>&</sup>lt;sup>b</sup>Department of Neuropathology, Royal Preston Hospital, Lancashire Teaching Hospitals NHS Trust, Preston PR2 9HT, UK

**Table S1:** A one-way ANOVA showing the differences between each of the normal, high-grade (HG) and low-grade (LG) glioma groups. Significance level p < 0.05.

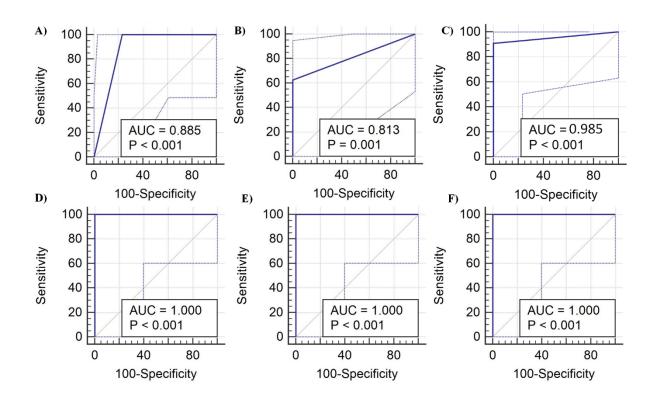
Tukey's multiple comparisons test	Mean Difference	95% CI of difference	Adjusted <i>P</i> -value
Normal vs. HG	0.05	0.05 to 0.06	< 0.0001
Normal vs. LG	0.01	0.01 to 0.02	< 0.0001
HG vs. LG	-0.04	-0.04 to	< 0.0001
		-0.03	

**Table S2:** Results of the one-way ANOVA showing statistically significant comparisons between each group. LG, low-grade glioma; HG, high-grade glioma; Mets, metastasis to brain. Significance level p < 0.05.

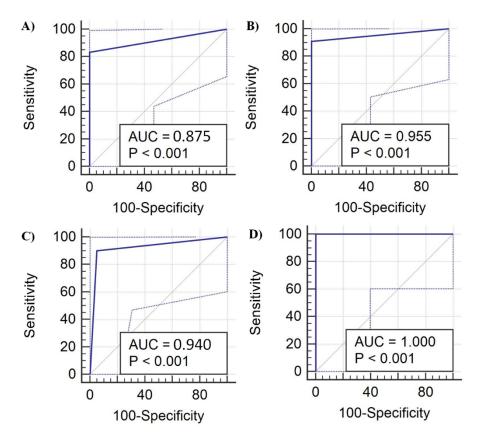
Tukey's multiple comparisons test	Mean Difference	95% CI of difference	Adjusted <i>P</i> -value
Normal vs. HG	0.05	0.05 to 0.06	< 0.0001
Normal vs. LG	0.01	0.01 to 0.02	< 0.0001
Normal <i>vs</i> . Meningioma	0.03	0.03 to 0.04	< 0.0001
Normal vs. Mets	0.02	0.02 to 0.03	< 0.0001
HG vs. LG	-0.04	-0.04 to -0.03	< 0.0001
HG vs. Meningioma	-0.02	-0.03 to -0.02	<0.0001
HG vs. Mets	-0.03	-0.04 to -0.02	< 0.0001
LG vs. Meningioma	0.02	0.01 to 0.02	< 0.0001
LG vs. Mets	0.01	0.00 to 0.01	0.0005
Meningioma vs. Mets	-0.01	-0.01 to -0.00	<0.0001



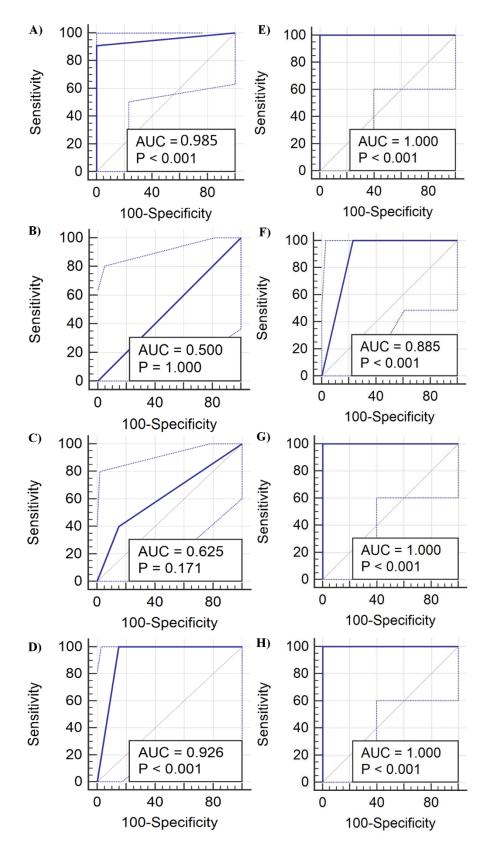
**Figure S1:** SVM optimization cost for (A) control *vs.* low-grade *vs.* high-grade gliomas; (B) control *vs.* meningioma; (C) control *vs.* metastasis; (D) control *vs.* colorectal adenocarcinoma *vs.* lung adenocarcinoma *vs.* melanoma; (E) control *vs.* low-grade glioma *vs.* high-grade glioma *vs.* meningioma *vs.* and metastasis; (F) control *vs.* low-grade glioma *vs.* high-grade glioma *vs.* meningioma *vs.* melanoma metastasis *vs.* colorectal adenocarcinoma metastasis *vs.* lung adenocarcinoma metastasis.



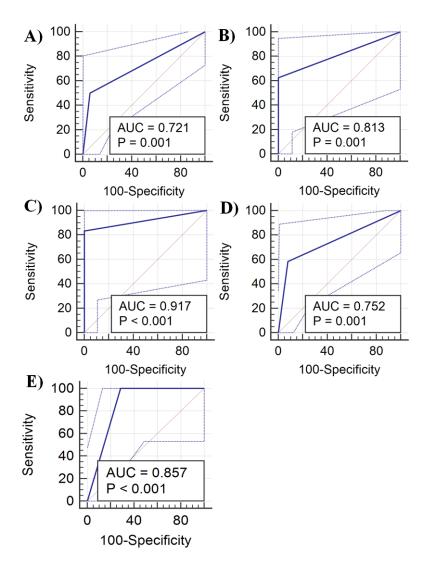
**Figure S2:** ROC curves for PCA-LDC in control (A) vs. low-grade (B) vs. high-grade (C) gliomas; and SVM in control (D) vs. low-grade (E) vs. high-grade (F) gliomas.



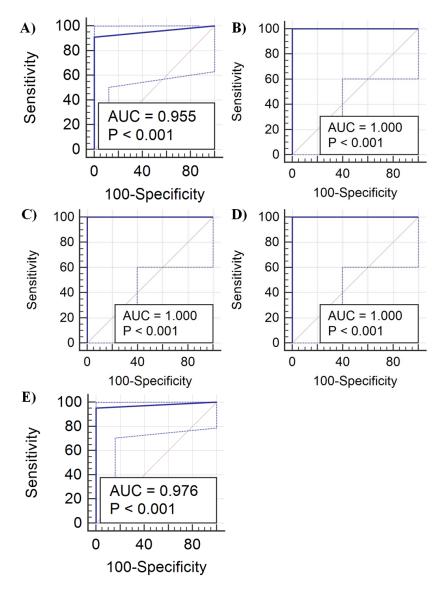
**Figure S3:** ROC curves for PCA-LDC (A) and SVM (B) in control *vs.* meningioma; and PCA-LDC (C) and SVM (D) in control *vs.* metastasis.



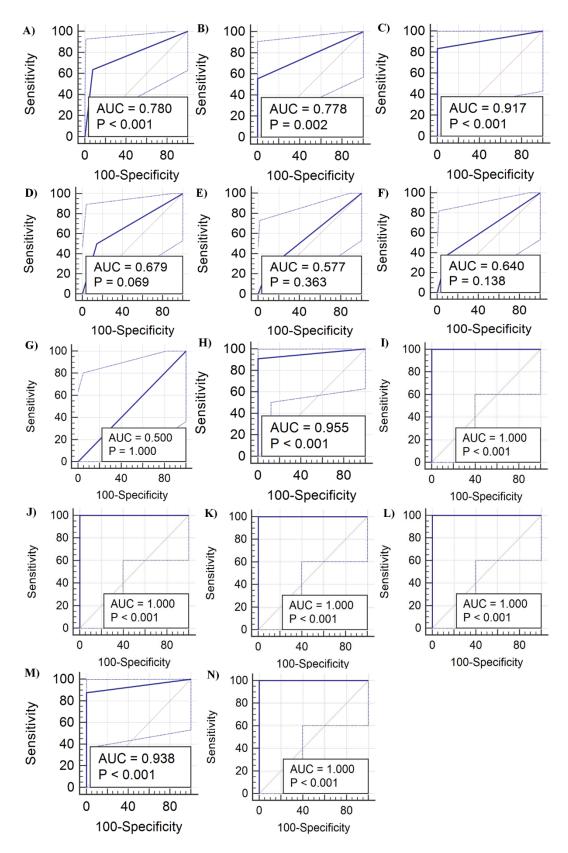
**Figure S4:** ROC curves for PCA-LDC in control (A), colorectal adenocarcinoma (B), lung adenocarcinoma (C), melanoma (D); and SVM in control (E), colorectal adenocarcinoma (F), lung adenocarcinoma (G), melanoma (H).



**Figure S5:** ROC curves for PCA-LDC in control (A), high-grade glioma (B), low-grade glioma (C), meningioma (D) and metastasis (E).



**Figure S6:** ROC curves for SVM in control (A), high-grade glioma (B), low-grade glioma (C), meningioma (D) and metastasis (E).



**Figure S7:** ROC curves for PCA-LDC in (A) control, (B) low-grade glioma, (C) high-grade glioma, (D) meningioma, (E) melanoma metastasis, (F) colorectal adenocarcinoma metastasis, (G) lung adenocarcinoma metastasis; and SVM in (H) control, (I) low-grade glioma, (J) high-grade glioma, (K) meningioma, (L) melanoma metastasis, (M) colorectal adenocarcinoma metastasis, (N) lung adenocarcinoma metastasis.