

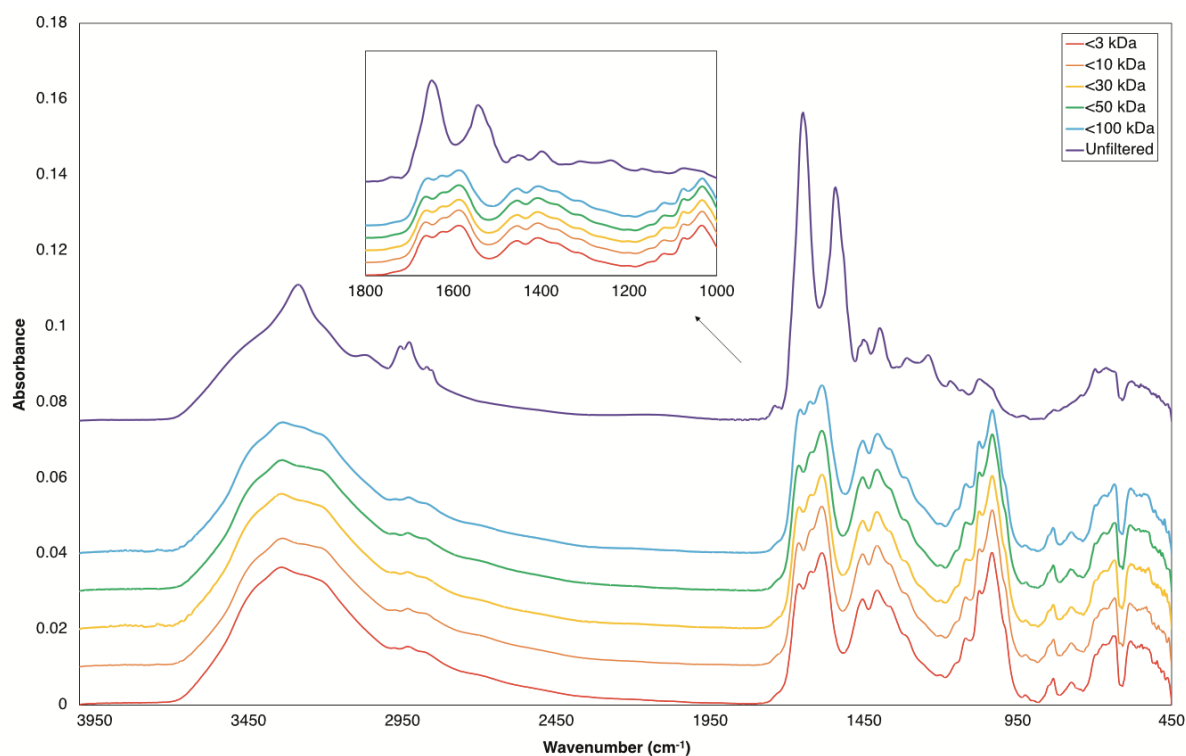
## Central Lancashire Online Knowledge (CLoK)

Title	Investigating centrifugal filtration of serum-based FTIR spectroscopy for the stratification of brain tumours
Type	Article
URL	<a href="https://clock.uclan.ac.uk/id/eprint/45316/">https://clock.uclan.ac.uk/id/eprint/45316/</a>
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Creators	Theakstone, Ashton, Brennan, Paul, Jenkinson, Michael, Goodacre, Royston and Baker, Matthew

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<https://doi.org/10.1371/journal.pone.0279669>

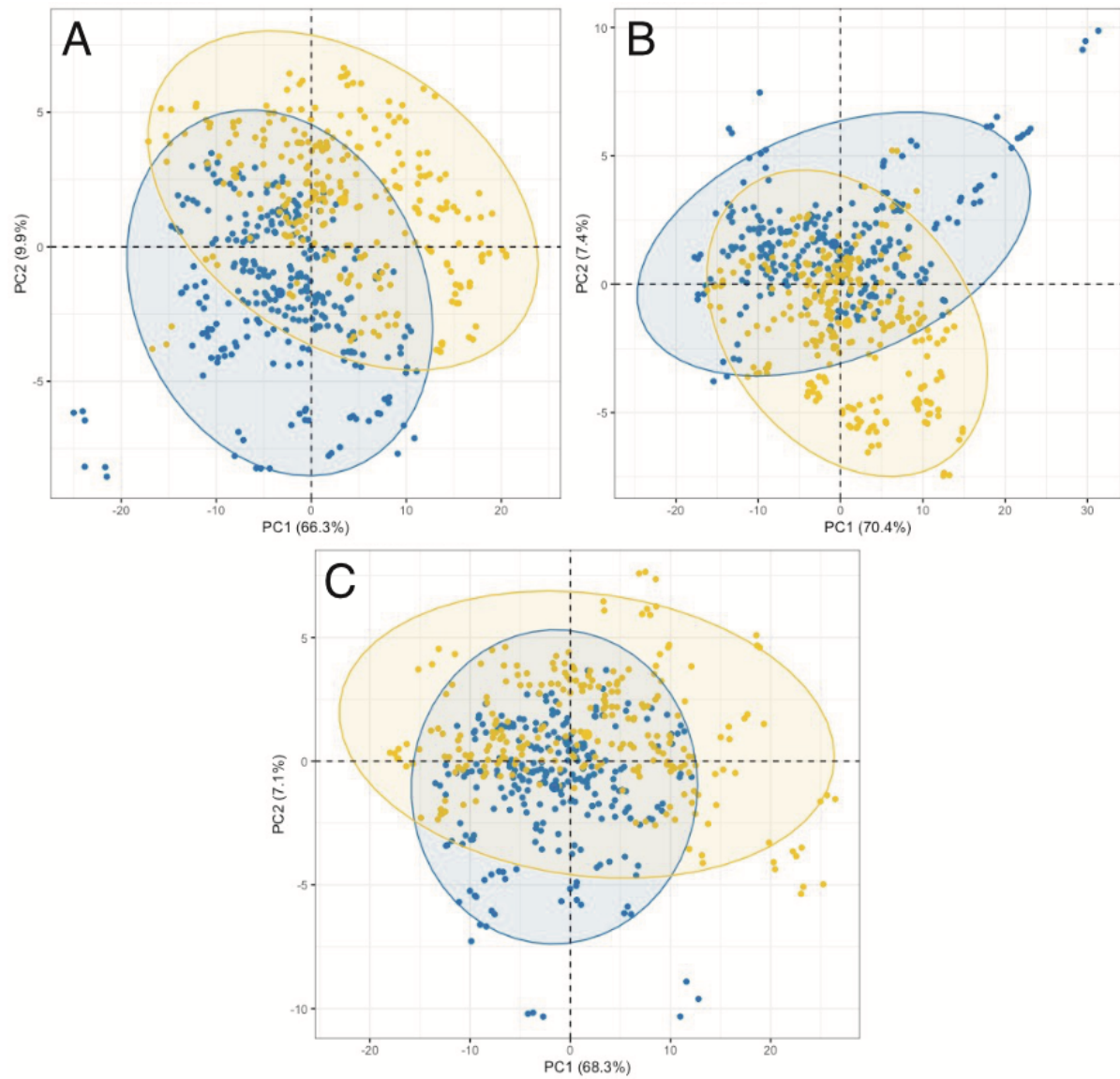
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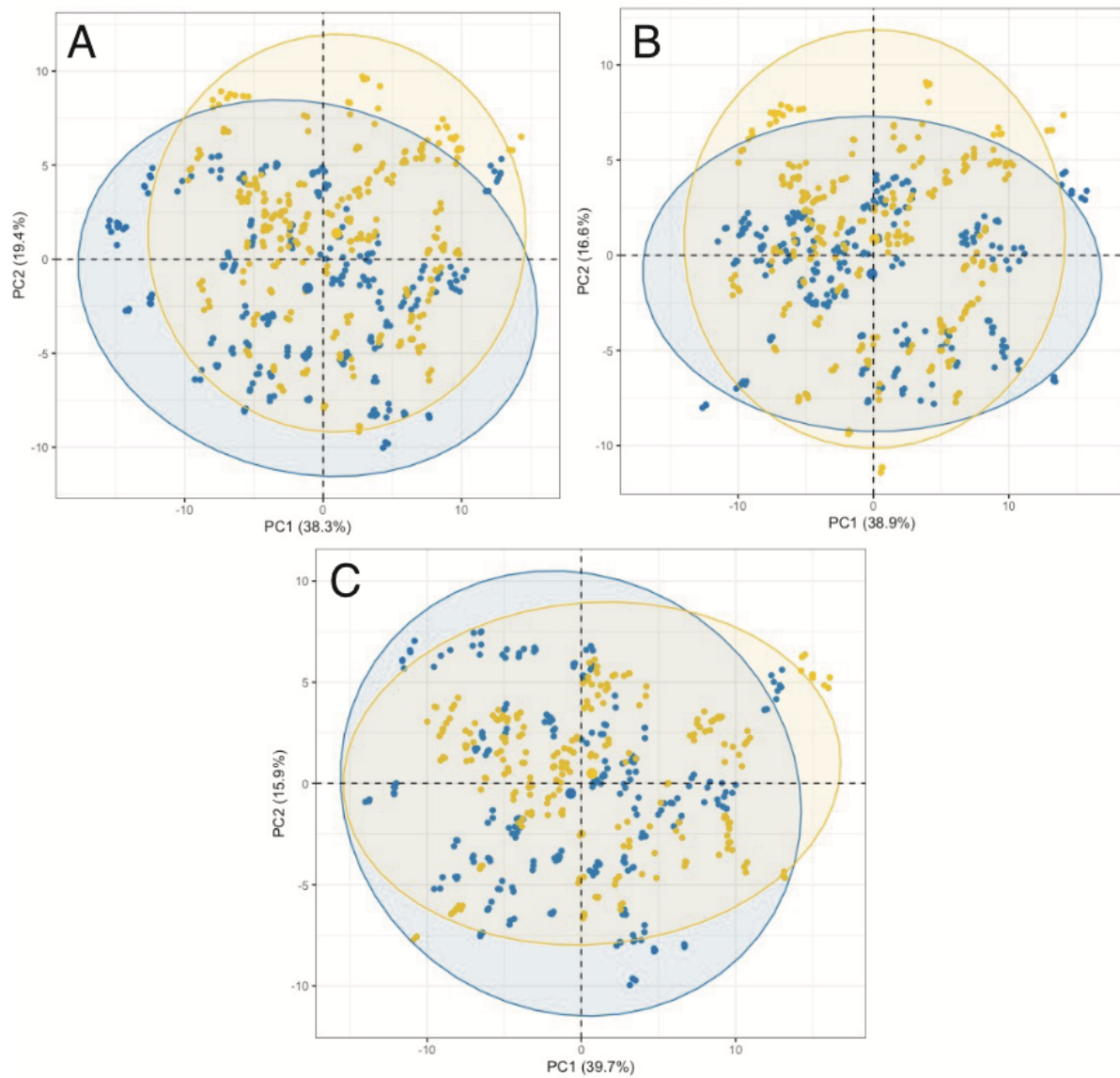
**Fig 1. Example of patient serum spectra including unfiltered whole serum and each molecular weight region.**

Average of the 30 GBM patients shown here. The inset is the wavenumber region between  $1800\text{ cm}^{-1}$  and  $1000\text{ cm}^{-1}$ , which was used for all chemometrics and machine learning analyses. Spectra is offset for clearer visualisation.

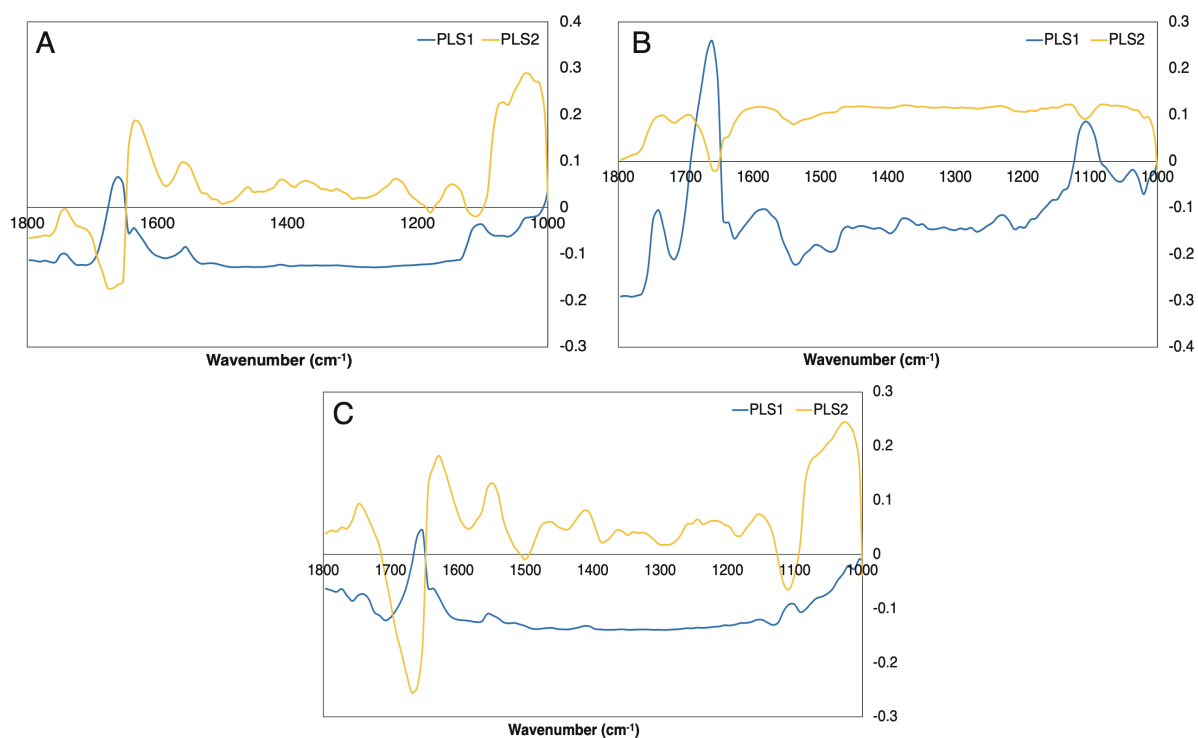


**Fig 2. Principal component analysis scores plots for the unfiltered whole serum of the first and second dimensions.**

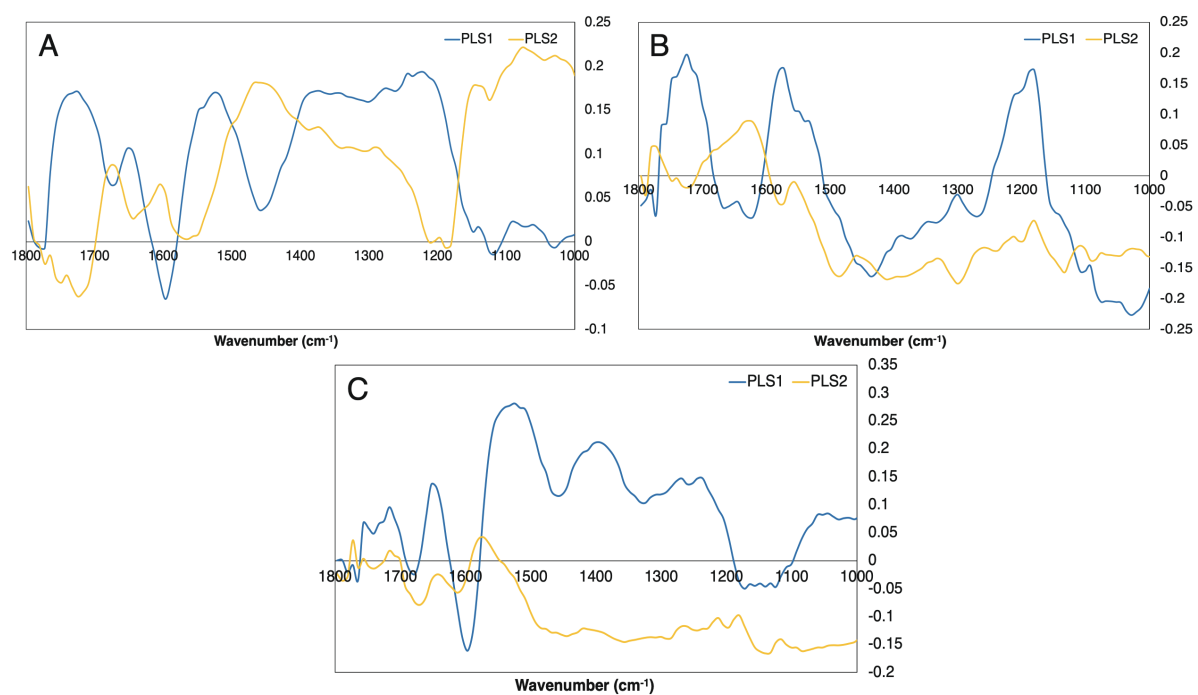
The three figures represent (A) GBM in blue and non-cancer in yellow, (B) lymphoma in blue and non-cancer in yellow and (C) GBM in blue and lymphoma in yellow. The eclipses in each class represent a 95% confidence interval. Values in parentheses within the axes legends are the total explained variance (TEV) for each principal component (PC).



**Fig 3. PCA scores plots for the filtered serum (<100 kDa) of the first and second dimensions.** The three figures represent (A) GBM in blue and non-cancer in yellow, (B) Lymphoma in blue and non-cancer in yellow and (C) GBM in blue and lymphoma in yellow. The eclipses in each class represent a 95% confidence interval. Values in parentheses are the TEV for each PC.



**Fig 4. PLS loadings plots for the 1<sup>st</sup> and 2<sup>nd</sup> latent variables (LVs) for the unfiltered whole serum.**  
 (A) GBM *versus* non-cancer, (B) Lymphoma *versus* non-cancer and (C) GBM *versus* lymphoma.



**Fig 5. PLS loadings plot for the 1<sup>st</sup> and 2<sup>nd</sup> LVs for the filtered serum (<100 kDa).**  
 (A) GBM *versus* non-cancer, (B) Lymphoma *versus* non-cancer and (C) GBM *versus* lymphoma.