

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Reduced list of m/z values revealed as main determinants of the molecular patterns captured in the latent space in the analysis of 5 different datasets.

File Name: Supplementary Data 2

Description: Peak list from the different cross-validation models.

File Name: Supplementary Data 3

Description: List of peaks identified by both msiPL and the OMP of the 3D MALDI MSI PDX GBM dataset.