

Stratification of tumour cell radiation response and metabolic signatures visualization with Raman spectroscopy and explainable Convolutional Neural Network

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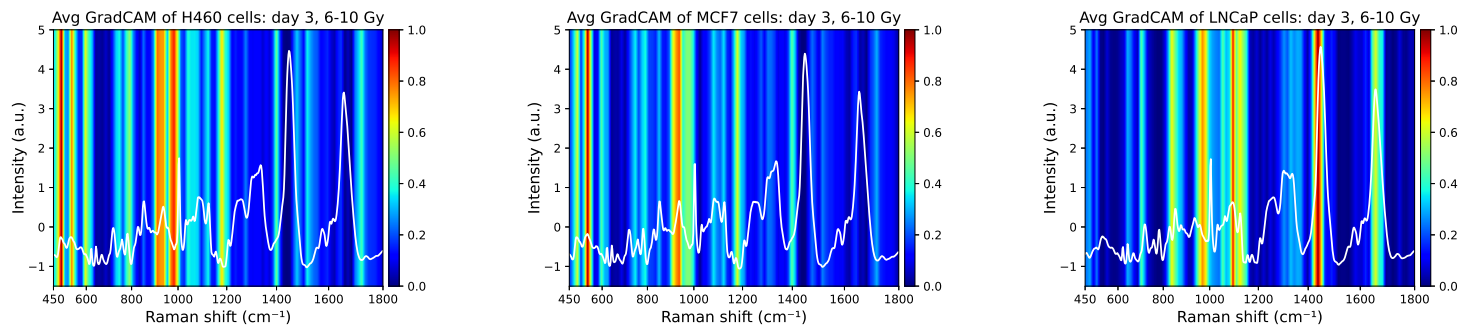
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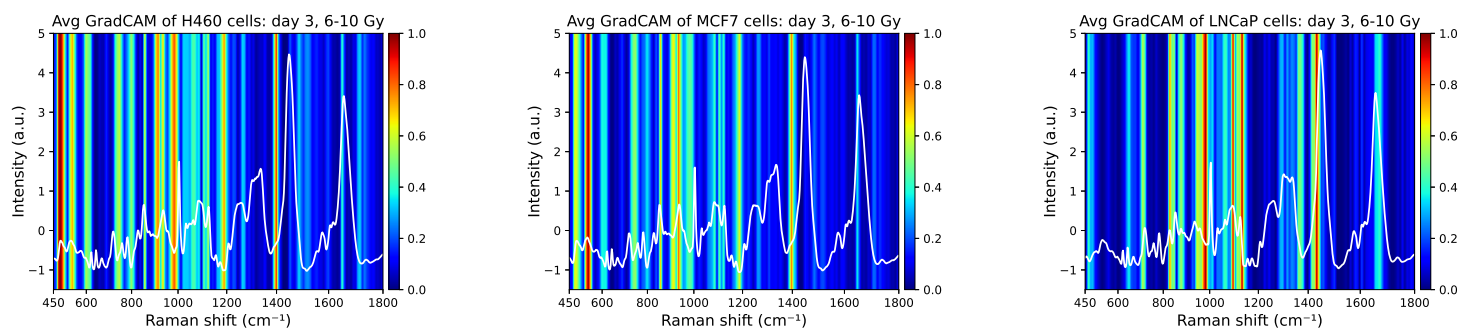
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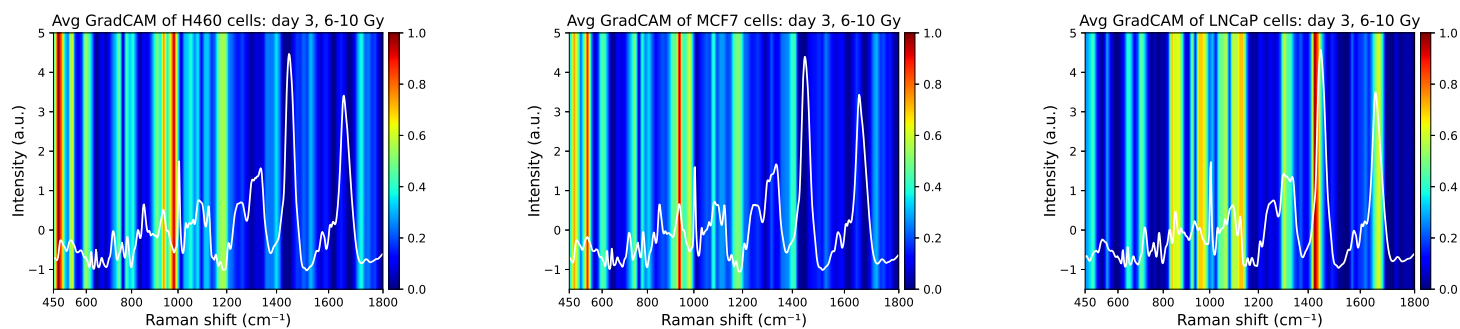
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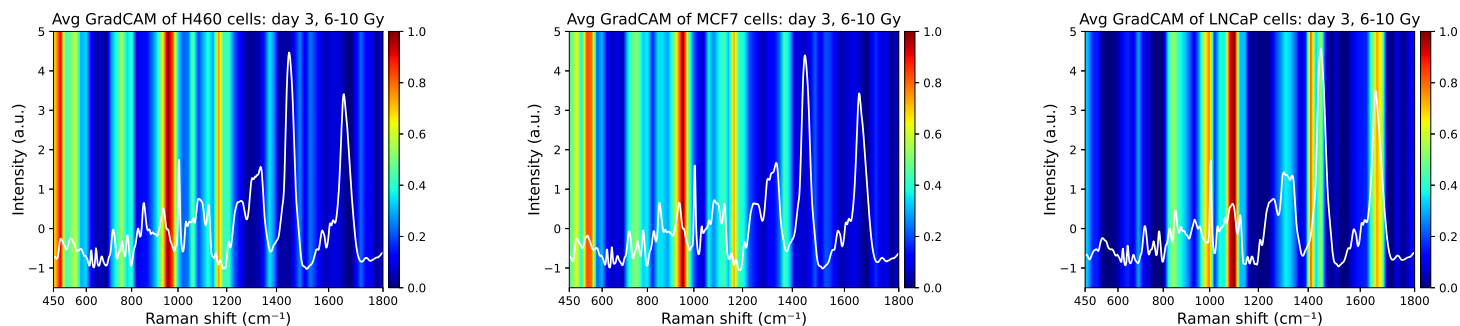
(a) Convolution filter numbers: 64 (first layer, stride 2), 64 (second layer, stride 3); filter size 7x1; 10-neuron fully connected layer before classification layer.



(b) Convolution filter numbers: 64 (first layer, stride 2), 64 (second layer, stride 2); filter size 5x1.



(c) Convolution filter numbers: 32 (first layer, stride 2), 32 (second layer, stride 3); filter size 6x1.



(d) Convolution filter numbers: 64 (first layer, stride 3), 128 (second layer, stride 3); filter size 7x1.

Figure S1. Grad-CAM saliency maps of H460, MCF7, and LNCaP cell Raman spectra exposed to single-fraction doses ranging 6-10 Gy and collected 3 days post-irradiation for four different CNN architectures, showing consistency in active peaks.

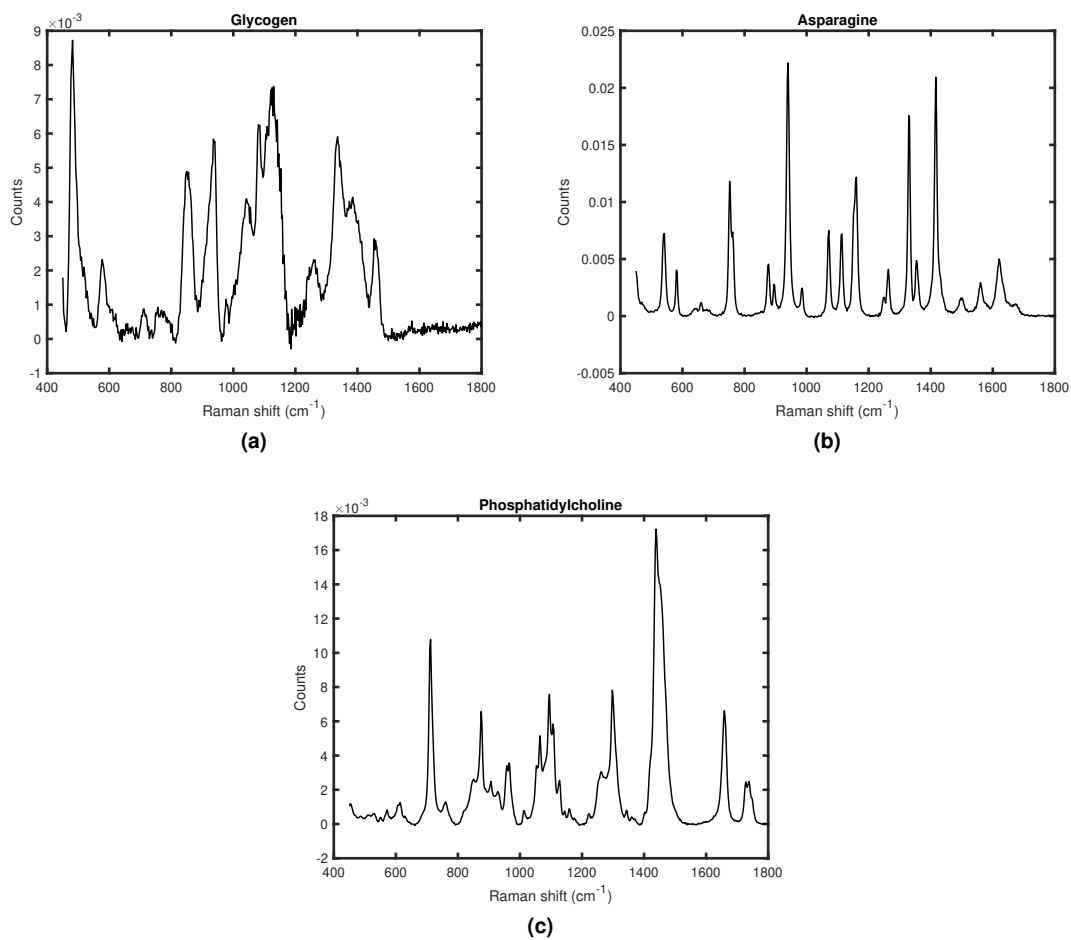


Figure S2. Raman spectra of (a)glycogen, (b)asparagine, and (c) phosphatidylcholine.