

Title: Raman spectroscopy identifies radiation response in human non-small cell lung cancer xenografts.  
 Authors: Harder, S.J., Isabelle, M., DeVorkin, L., Smazynski, J., Beckham, W., Brolo, A.G., Lum, J.J., Jirasek, A.

## Supplemental material

Supplementary Table S.1: Raman peak assignment for radiation induced principal component 1 (PC1). Only main spectral contributors to the PC are listed. Italicised assignments indicate negative PC features.

Raman Shift (cm <sup>-1</sup> )	Assignment		
	Protein	Lipid	Carbohydrate
482			<i>glyc.</i>
580			<i>glyc.</i>
729		C-N h.g. <sup>1</sup>	
815		O-P-O <sup>1</sup>	
850			<i>glyc.</i>
940			<i>glyc.</i>
980		C-C h.g. <sup>1</sup>	
1042			<i>glyc.</i>
1083			<i>glyc.</i>
1129			<i>glyc.</i>
1240	Amide III r.c. <sup>1</sup>		
1245	Amide III β sheet <sup>1</sup>		
1274	Amide III β sheet <sup>1</sup>	=CH def. <sup>1</sup>	
1284	Amide III α helix <sup>1</sup>	=CH def. <sup>1</sup>	
1297		CH <sub>2</sub> tw. <sup>1</sup>	
1338			<i>glyc.</i>
1385			<i>glyc.</i>

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<b>Assignment</b>			
<b>Raman Shift (cm<sup>-1</sup>)</b>	<b>Protein</b>	<b>Lipid</b>	<b>Carbohydrate</b>
1447	CH def. <sup>1</sup>	CH def. <sup>1</sup>	
1465	CH def. <sup>1</sup>	CH def. <sup>1</sup>	
1661	Amide I $\alpha$ helix <sup>1</sup>	C=C str. <sup>1</sup>	

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glyc. - glycogen, h.g. - head groups, r.c. – random coil, def. - deformation, tw. - twist, str. - stretch.

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Supplementary Table S.2: Raman peak assignment for principal component 2 (PC2). Only main spectral contributors to the PC are listed. Italicised assignments indicate negative PC features.

Raman Shift (cm <sup>-1</sup> )	Assignment		
	Nucleic Acid	Protein	Lipid
669	G, T <sup>2</sup>		
716			<i>Cho.</i> <sup>2</sup>
729	A <sup>1</sup>	Trp. <sup>1</sup>	
784	T <sup>1</sup>		
825			<i>Cho.</i> <sup>3</sup>
937		<i>C-C bk. str. α helix</i> <sup>1</sup>	
1004		Phe. <sup>1</sup>	
1047		Phe. <sup>2</sup>	
1066		<i>C-N str.</i> <sup>1</sup>	<i>Chain C-C str.</i> <sup>1</sup>
1080		<i>C-N str.</i> <sup>1</sup>	<i>Chain C-C str.</i> <sup>1</sup>
1087			<i>Chain C-C str.</i> <sup>1</sup>
1127		<i>C-N str.</i> <sup>1</sup>	<i>Chain C-C str.</i> <sup>1</sup>
1180		Phe. <sup>2</sup>	
1210		Phe., Trp. <sup>1</sup>	
1272			<i>=CH def.</i> <sup>2</sup>
1284		<i>Amide III α helix</i> <sup>1</sup>	<i>=CH def.</i> <sup>1</sup>
1301			<i>CH<sub>2</sub> tw.</i> <sup>1</sup>
1328	G <sup>1</sup>		
1338		Trp. <sup>4</sup>	

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Raman Shift (cm <sup>-1</sup> )	Assignment		
	Nucleic Acid	Protein	Lipid
1342	A, G <sup>1</sup>		
1365	T <sup>2</sup>		Sym. str. CH <sub>3</sub> <sup>1</sup>
1374	A, G <sup>5</sup>	Trp. <sup>4</sup>	
1450		CH def. <sup>1</sup>	CH def. <sup>1</sup>
1460		CH def. <sup>1</sup>	CH def. <sup>1</sup>
1576	A, G <sup>5</sup>	Trp. <sup>4</sup>	
1607		Phe. <sup>1</sup>	
1621		Trp. <sup>1</sup>	
1659		Amide I $\alpha$ helix <sup>1</sup>	C=C str. <sup>1</sup>
1740			>C=O ester <sup>1</sup>

cho. – choline, bk. - backbone G - guanine, A - adenine, T - thymine, Phe. - phenylalanine, Trp.

- tryptophan, def. – deformation, tw. – twist, sym. – symmetric, str. – stretch.

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## References:

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