

Supporting Information for:

Identifying the lineages of individual cells in cocultures by multivariate analysis of Raman spectra

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Supplemental Figures and Tables

Table 1. Peak assignments for Raman spectra of live cells

Peak Position (cm ⁻¹)	Nucleic Acids	Proteins	Lipids	Carbohydrates
623		C-C twist Phe ¹		
645		C-C twist Tyr ¹		
669	T,G ¹			
677	G ²			
728	A ¹			
748	T ²			
783	U,C,T ring br. ¹			
811			O-P-O ¹	
828	O-P-O str. ¹	Out of plane ring br. Tyr ¹		
853		Ring br. Tyr ¹		
897	BK, deoxyrib. ¹			
937		C-C BK str. α helix ¹		C-O-C glycos. ¹
957		CH ₃ def. ³	CH ₃ def. ³	
985			C-C head groups ¹	
1005		Sym. ring br. Phe ¹		
1013	C-O deoxyrib. ¹			
1033		C-H in-plane Phe ¹		
1046		Cell culture media (undefined) ⁴		
1066		C-N str. ¹		C-O, C-C str. ¹
1080		C-N str. ¹		
1128		C-N str. ¹		C-O str. ¹
1158		C-C/C-N str. ²		
1175		C-H in-plane bend Tyr ¹		
1209		C-C ₆ H ₅ str. Phe, Trp ¹		
1258		C-C/C-N str. ¹		
1301			CH ₂ twist ¹	

1319	G ¹	CH def. ¹		
1336	G,A ²	CH def. ²		
1367			Sym. Str. CH ₃ ¹	
1421	G,A ²			
1449		CH def. ¹	CH def. ¹	CH def. ¹
1510	A ²			
1551		Amide II C=O str. ³		
1575	G,A ²			
1607		C=C Phe, Tyr ¹		
1617		C=C Tyr, Trp ¹		
1659		Amide I α helix ¹	C=C str. ¹	

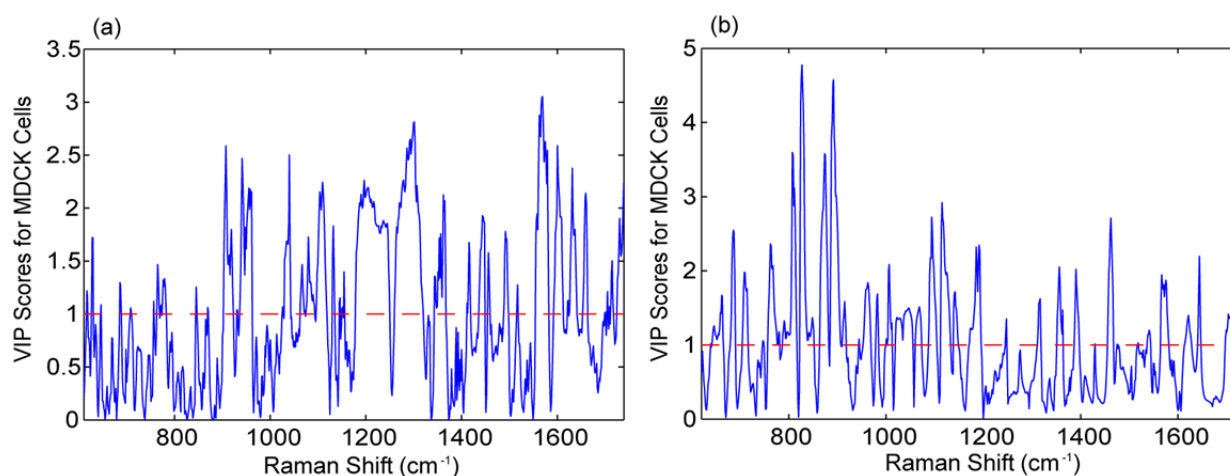


Figure S1. Variable importance in prediction (VIP) plots for PLS-DA models constructed for fixed (a) and live (b) cells in coculture. Peaks with VIP scores greater than unity are important for distinguishing MDCK from CHO-K1 cells. The most valuable peaks in the fixed cell PLS-DA model correspond to 1575 cm⁻¹ (DNA: G, A), 897cm⁻¹ (DNA: deoxyribose), and 1301 cm⁻¹ (lipids: CH₂ twist). The most valuable peaks in the live cell PLS-DA model corresponded to 828 cm⁻¹ (DNA: O-P-O stretch, protein: Tyr.), and 852 cm⁻¹ (protein: Tyr). The peak at 1046 cm⁻¹, corresponding to the cell media, did not have a high VIP score in the live cell model. Removal of this peak from data set produced insignificant changes in the error of identification for the cells in “quasi” coculture and coculture, confirming that contributions from cell media have a minimal effect on cell identification.

REFERENCES

1. I. Notingher, S. Verrier, S. Haque, J. M. Polak and L. L. Hench, *Biopolymers*, 2003, **72**, 230-240.
2. J. W. Chan, D. S. Taylor, T. Zwerdling, S. M. Lane, K. Ihara and T. Huser, *Biophys. J.*, 2006, **90**, 648-656.
3. C. Aksoy and F. Severcan, *Spectrosc. Int. J.*, 2012, **27**, 167-184.
4. P. V. Zinin, A. Misra, L. Kamemoto, Q. Yu, N. Hu and S. K. Sharma, *J. Raman Spectrosc.*, 2010, **41**, 268-274.