



Supporting Information

Lipidome profiling with Raman microspectroscopy identifies macrophage response to surface topographies of implant materials

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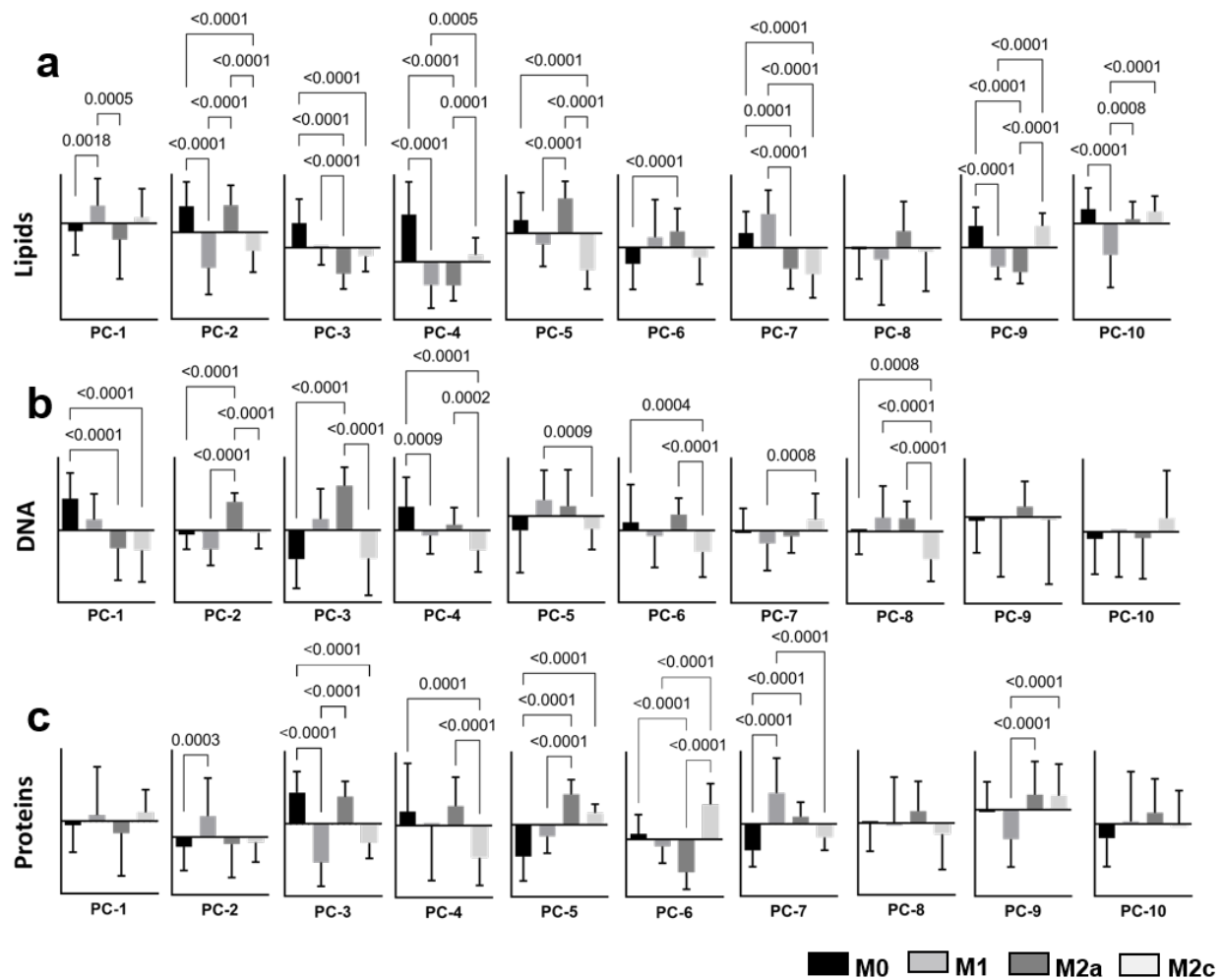
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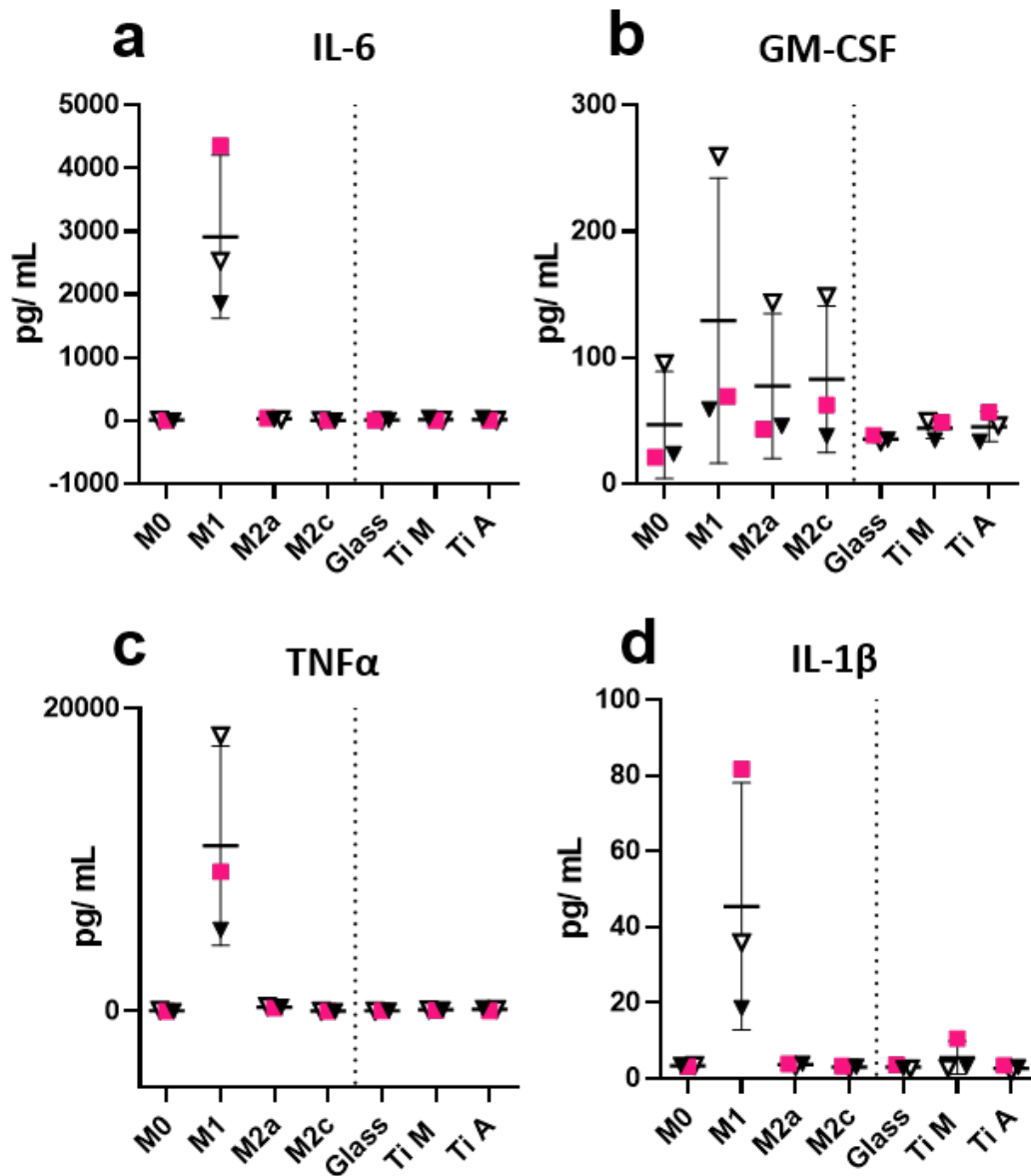
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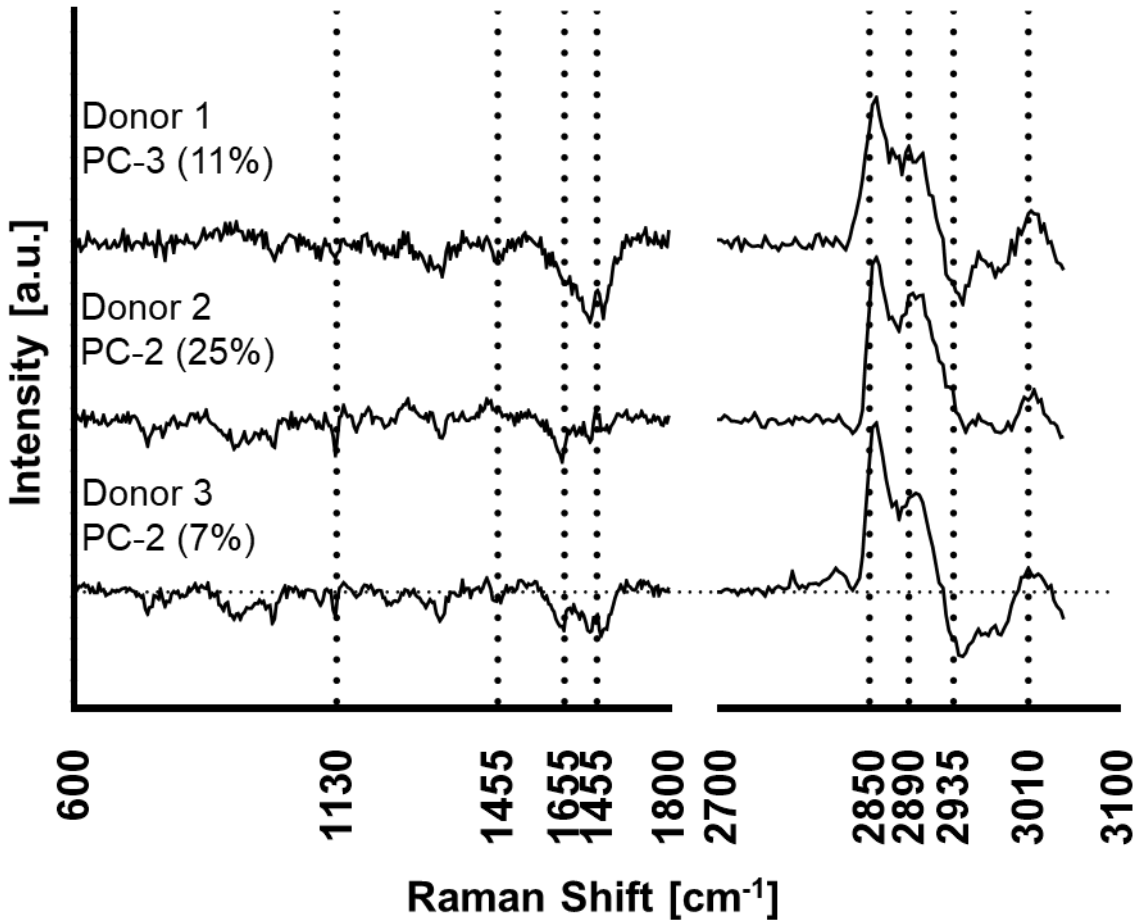
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Supporting Figure 1. Analysis of PCA scores of major cell components helps identifying optimal separation of MDM subtypes. First 10 principal components of (a) lipids, (b) nucleic acids, and (c) proteins were analyzed for significance using Kruskal-Wallis + Dunn's post hoc test. Scores are plotted as mean \pm SD. Each subtype contains data of 30 cells from each donor (total of 180 cells).



Supporting Figure 2. Expression of inflammation-associated cytokines is not increased on glass and titanium. To assess activation status of MDMs cultured on biomaterial surfaces, inflammation-associated cytokines were analyzed by multiplex bead immuno-sandwich assay. IL-6 (a), GM-CSF (b), TNFα (c), and IL-1β (d) did not show increased expression compared to M0 MDMs.



Supporting Figure 3. Loadings plots indicate comparable biochemical changes occurring in all donors in MDMs adherent to biomaterials. To assess if Raman spectral information can be used to identify MDM polarization in individual donors, direction vectors that define the multivariate model need to be compared. Here, the original variables have comparable loadings, indicating that separation is based on similar biochemical changes within the cell.

Supporting Table 1. Raman peaks of MDM components and their associated molecular assignments.

Peak [cm^{-1}]	Molecular Assignment	Component	Reference
748	Ring breathing vibrations of nucleic acids and tryptophan	DNA	[7, 8]
923	C-H stretch of proline	Proteins	[9]
935	A-helix	Protein	[4, 8]
1005	Symmetric ring breathing of Phenylalanin (Phe)	Protein	[4, 8]
1100	PO_2^-	DNA	[2, 8]
1127	C-N stretching	Proteins	
1235	extended Amide III, peptide backbone	Proteins	[4]
1270	$=\text{CH}_2$, C=C in USFA	Lipids	[9]
1310	CH_3CH_2 twisting mode	Lipids	[8]
1340	Adenin	DNA	[4]
1350	Thymine, Adenine, Guanine	DNA	[4]
1440	CH_3/CH_2 scissoring, CH_2 deformation	Lipids	[8, 9]
1450	CH_2 bending	Proteins	[9]
1585	C=C olefinic stretch	Proteins	[9]
1655	C=C lipid stretch	Lipids	[4, 8]
2850 - 2855	$=\text{CH}_2$, symmetric stretching	Lipids	[9]
2886 - 2895	$=\text{CH}_2$, asymmetric stretching	Lipids	[9]
2920 - 2935	$=\text{CH}_3$, symmetric stretching	Lipids	[9]
2950	$=\text{CH}_3$, asymmetric stretching	Lipids	[9]
2980	CH stretching	Lipids	[9]
3005 - 3020	$=\text{CH}$ stretching of USFA	Lipids	[9]