

Fig. b. Figure of principal component (PC) analysis scores plot, representing the nuclear magnetic resonance spectrum of an individual human synovial fluid sample and demonstrating that the tendency for separation is driven by the presence of infection rather than joint type (native or prosthetic). Data were scaled to unit variance. The percentage variation explained is 38% for PC1 and 21% for PC2.

Table i. Table of metabolites from both infected and noninfected synovial fluid consistently identified in all samples.

Metabolite	Chemical shift (ppm)
Cholesterol (C18)	0.58 (bs), 0.65 (bs)
CH3 (fatty acyl residues, lipids)	0.85 (bs)
CH2 (fatty acyl residues, lipids)	1.25 (bs)
Isoleucine	0.93 (t), 1.00 (d), 1.25 (m), 1.46 (m), 1.96 (m), 3.66 (d)
Leucine	0.95 (d), 0.96 (d), 2.00 (m)
Valine	0.98 (d), 1.03 (d), 2.26 (m), 3.60 (d)
3-Hydroxyisobutyrate	1.06 (d), 2.48 (m)
3-Hydroxybutyrate	1.19 (d), 2.35 (dd), 4.14 (m)
Lactate	1.32 (d), 4.10 (q)
Alanine	1.47 (d), 3.78 (q)
Lysine	1.47 (m), 1.71 (m), 1.89 (m), 3.03 (t), 3.72 (t)
Arginine	1.69 (m), 1.90 (m), 3.23 (t)
Acetate	1.91 (s)
GAGs	2.02 (s), 3.34 (bs), 4.46 (bs), 7.97 (bs)
N-acetyl groups (glycoproteins)	2.04 (bs)
Glutamate	2.06 (m), 2.34 (m)
Acetone	2.22 (s)
Pyruvate	2.37 (s)
Glutamine	2.12 (m), 2.45 (m), 3.74 (dd)
Citrate	2.53 (d), 2.67 (d)
Creatine	3.03 (s), 3.91 (s)
Creatinine	3.04 (s), 4.05 (s)
Dimethylsulfone	3.14 (s)

Choline	3.19 (s)
Glucose	3.23 (dd), 3.46 (dd), 3.49(t), 3.53 (dd), 3.71 (t), 3.72 (dd), 3.76 (dd), 3.82(m), 3.85(m), 3.90 (dd), 4.64 (d), 5.23 (d)
Proline	3.34 (m)
Glycine	3.55 (s)
Mannose	5.18 (d)
CH=CH (fatty acyl residues, lipids)	5.28 (bs)
Tyrosine	6.89 (d), 7.19 (d)
Histidine	7.05 (s), 7.77 (s)
Formate	8.45 (s)

bs, broad singlet; d, doublet; dd, doublet of doublets; GAG, glycosaminoglycan; m, multiplet; ppm, parts per million; q, quartet; s, singlet; t, triplet.

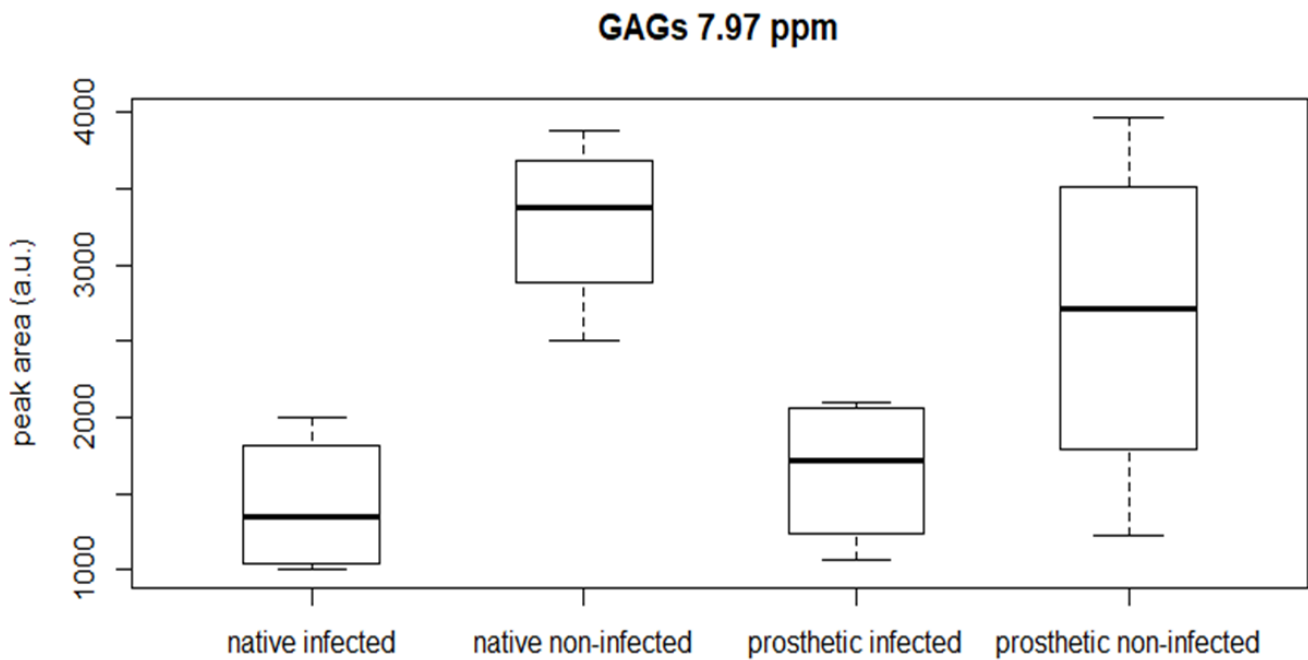


Fig. c. Boxplot demonstrating differences in the levels of glycosaminoglycans (GAGs) in the native and prosthetic subgroups, when comparing infected and noninfected synovial fluid. This demonstrates lower concentrations of GAGs in the infected groups, which appears independent of whether the joint was native or prosthetic.

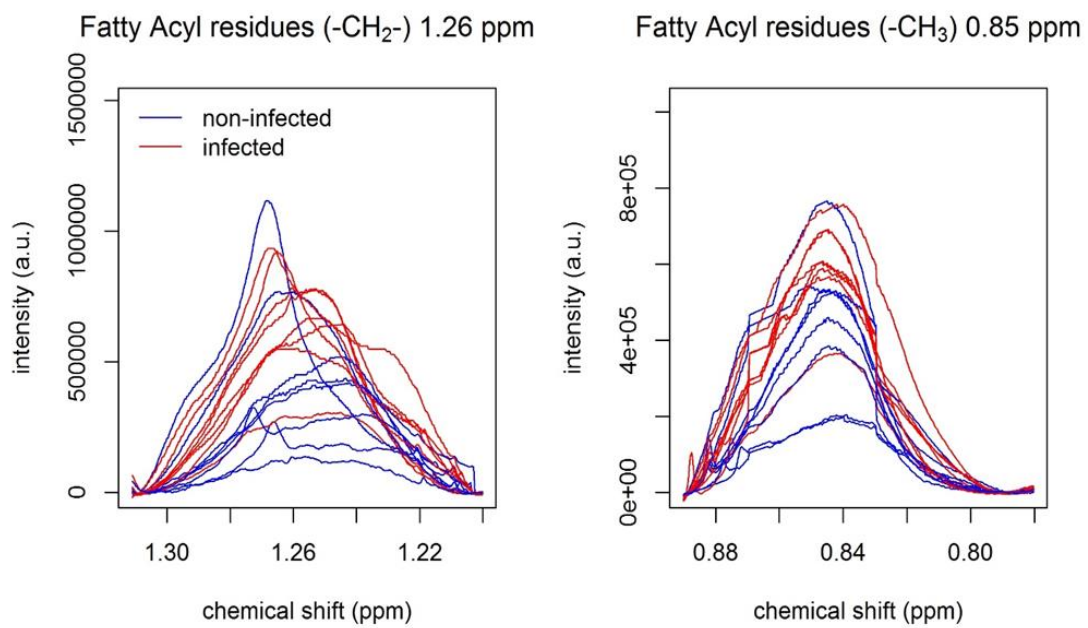


Fig. d. Further metabolite analysis from spectral inspection of the remaining fatty acyl residue regions. This figure demonstrates the same trend in peak intensities for both the infected (red) and noninfected (blue) synovial fluid samples. The p-values are 0.068 (0.85 parts per million (ppm)) and 0.051 (1.26 ppm).