

Supplementary Material

Table A Summary of instrumentation parameters

Thermal desorber	
Primary desorption flow	50cm ³ min ⁻¹
Primary split	Splitless
Primary desorption temperature	180°C
Primary desorption time	5 min
Cold trap volume	19 µl
Cold trap temperature	-10° C
Cold trap packing	Tenax TA/Carbograph 1TD
Secondary desorption flow	1cm ³ min ⁻¹
Secondary split	50:1
Trap heating rate	100°C min ⁻¹
Secondary desorption temperature	300°C
Secondary desorption time	3min
Gas Chromatograph	
Column flow	1cm ³ min ⁻¹
Initial column temperature	70 °C
Time that initial column temperature was held	1min
Column heating rate	3°C min ⁻¹
Final Column temperature	230°C
Time that final column temperature was held	10 min
Ion Trap Mass Spectrometer	
Ionisation EI mode	10µA
Scan range	30 to 400m/z
Scan time	1s
Trap temperature	200°C
Manifold Temperature	90°C
Transfer line temperature	260°C
Filament and Multiplier delay	30s

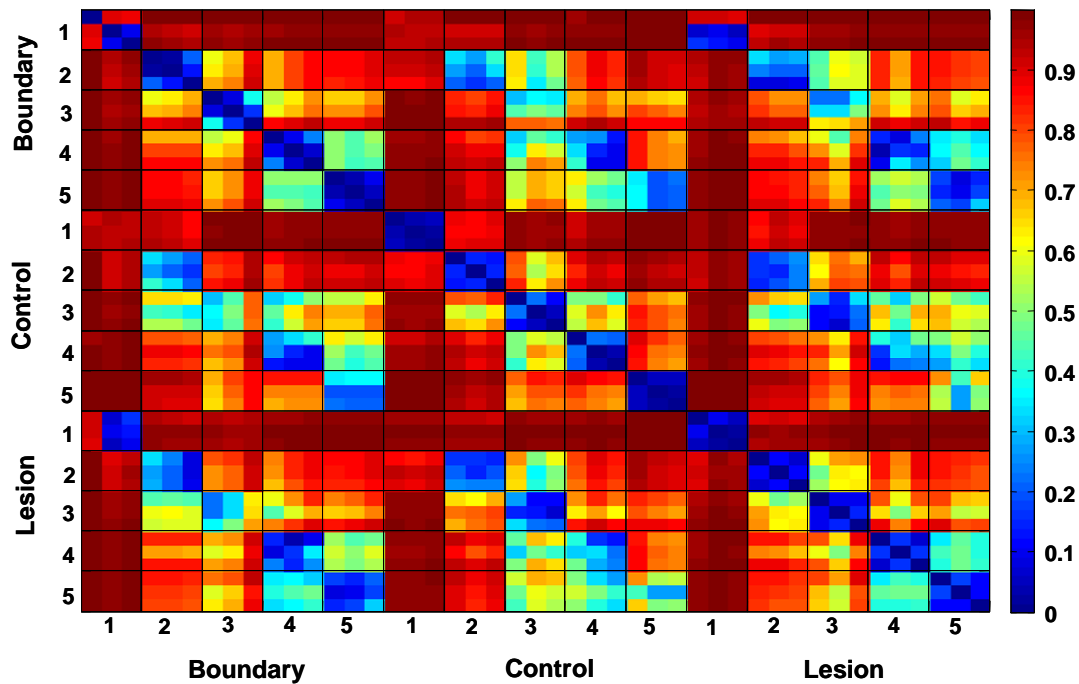


Figure 6. Distance heat map plot. The distance between each pair of samples are represented by a colour as indicated by the colour bar on right (red to blue). The higher the distance, the lower (bluer) the similarity between two samples. The 5 different subjects, each subject has 3 samples from each class respectively, were labeled by numbers from 1-5 and samples from the sample class (e.g. Boundary, Control or Lesion) were placed together. Since each subject has 3 samples for each class, the 3x3 blocks in the diagonal of the picture represent the similarities between the samples from the same subject and also the same class which thereby show the reproducibility of the sampling methodology.