

SUPPLEMENTARY MATERIAL

Comparison of GC-MS, HPLC-MS and SIFT-MS in Conjunction with Multivariate Classification for the Diagnosis of Crohn's Disease in Urine

Michael Cauchi^{1*}, Dawn P. Fowler², Christopher Walton², Claire Turner³, Rosemary H. Waring⁴,
David B. Ramsden⁴, John O. Hunter⁵, Phil Teale⁶, Jeffrey A. Cole⁴ & Conrad Bessant⁷

¹School of Aerospace, Transport and Manufacturing, Cranfield University, Bedfordshire MK43 0AL, UK

²School of Energy, Environment and Agrifood, Cranfield University, Bedfordshire MK43 0AL, UK

³The Department of Life, Health and Chemical Sciences, Open University, Milton Keynes, MK7 6AA, UK

⁴School of Biosciences, University of Birmingham, Birmingham B15 2TT, UK

⁵Gastroenterology Research Unit, Box 262, Addenbrooke's Hospital, Cambridge CB2 0QQ, UK

⁶LGC, Newmarket Rd, Fordham, Cambridgeshire CB7 5WW, UK

⁷School of Biological and Chemical Sciences, Queen Mary University of London, Mile End Road, London E1 4NS, UK

* Corresponding author

***Dr Michael Cauchi**, Research Fellow, Centre for Biomedical Engineering, School of
Aerospace, Transport and Manufacturing, Building 63, Cranfield University, Cranfield,
Bedfordshire MK43 0AL, UK.

**Tel (Direct): +44 7917 589 126; Tel (General): +44 (0)1234 750111; Email:
m.cauchi@cranfield.ac.uk**

SUPPLEMENTARY MATERIAL

Supplementary Material

S1: HPLC-MS Instrumental Parameters

Table SM1. Summary of instrumental setup for HPLC-MS data acquisition

Column	Waters 100 mm × 2.1ID 3µm Atlantis T3		
Guard Column	Phenomenex Security Guard, C18		
Solvent A	0.1% Acetic acid in water with 300µg/litre uracil		
Solvent B	0.1% acetic acid in acetonitrile with 300µg/litre uracil		
Injection	10µl, no waste, wash solvent - water		
Autosampler	10 °C with a wait time pre run of 1.70 min		
Column Temp.	35 °C		
Gradient			
Time (mins)	% Solvent A	% Solvent B	Flow rate (µl/min)
0	100	0	400
1.20	90	10	400
2.00	65	35	400
3.00	35	65	400
3.50	2	98	400
4.50	2	98	400
4.51	100	0	400
Mass Spectrometry			
Source Type	Electrospray ionisation (ESI) – positive polarity		
Capillary Temp (°C)	200.00		
Sheath Gas Flow	30.00 (arbitrary units)		
Aux Gas Flow	10.00 (arbitrary units)		
Ion Trap Zoom AGC Target	3000.00		
Ion Trap Full AGC Target	30000.00		
FTMS Full AGC Target	500000.00		
FTMS SIM AGC Target	10000.00		
FTMS MSn AGC Target	200000.00		
Source Voltage (kV)	4.50		
Source Current (µA)	100.00		
Capillary Voltage (V)	36.00		
Tube Lens (V)	90.00		
Divert Time (min)	0.00 To Waste		
Divert Time (min)	0.50 To Source		