

Supporting Information for Publication for:

Characterisation of a micro-plasma for Ambient Mass Spectrometry Imaging

Andrew Bowfield,^{*a,b} Josephine Bunch,^b Tara L. Salter,^b Rory T. Steven,^b Ian S. Gilmore,^b Dave A. Barrett,^c Morgan R. Alexander,^c Kirsty McKay^a and James W. Bradley^a

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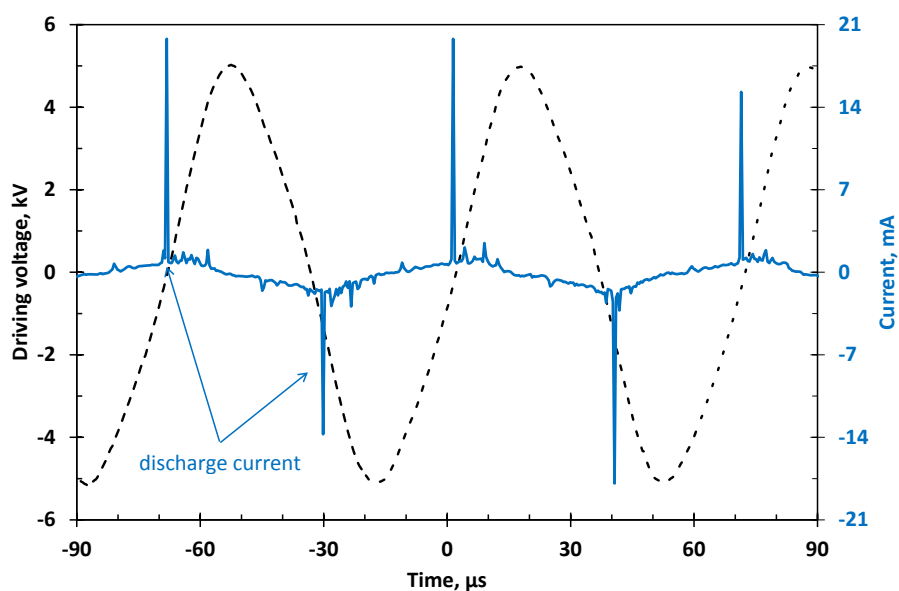


Figure S1. *IV* graph displaying the variation in the discharge current (solid line, right-hand axis) as a function of the applied sinusoidal driving voltage (dashed line, left-hand axis). The peak-to-peak voltage is approximately 10 kV. The spikes in the discharge current, which appear periodically with the applied voltage and twice in very waveform, are representative of the creation and ejection of the ‘plasma bullets’ from the electrode within the capillary.

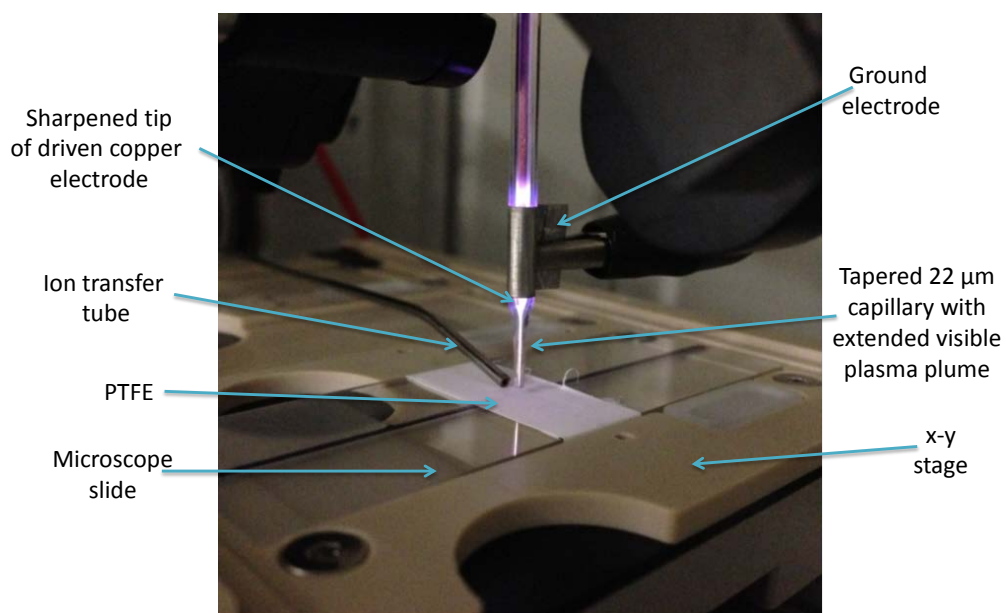


Figure S2. An optical image of the micro-plasma device in operation with major components labelled.

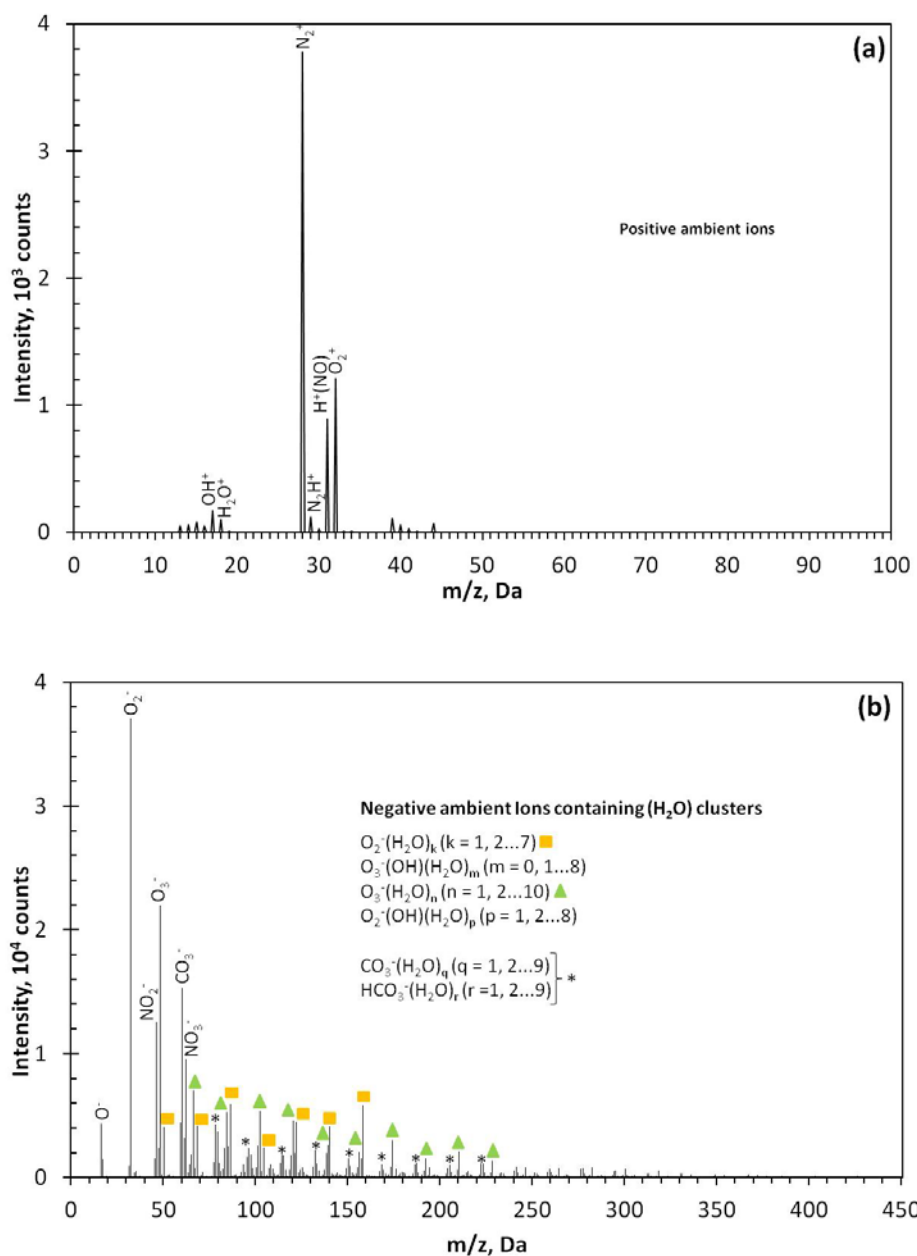


Figure S3. The (a) positive and (b) negative ambient ions detected using a Hiden Analytical HPR-60 MBMS, produced as a result of plasma/air interactions using a 56 μ m diameter capillary.

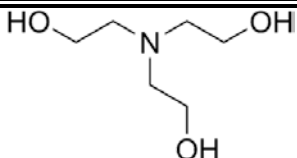
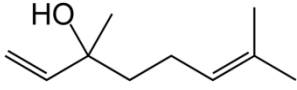
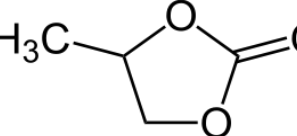
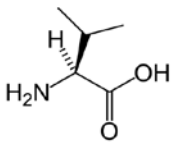
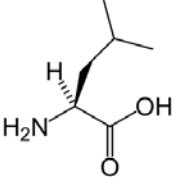
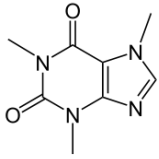
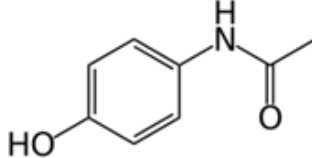
	Substance	Molecular formula	Mass, Da	Structure	Type of Substance	Positive ion mode (Dominant ion in bold)
P C P	Triethanol-amine	C ₆ H ₁₅ O ₃ N	149.11		Liquid	[M+H]⁺ = 150 [M+H-H ₂ O] ⁺ = 132
	Linalool	C ₁₀ H ₁₈ O	154.14		Liquid	[2M+H-2(H₂O)]⁺ = 273
	Propylene carbonate	C ₄ H ₆ O ₃	102.03		Liquid	[2M+H]⁺ = 205 [M+H] ⁺ = 103
A M I N O A C I D S	Valine	C ₅ H ₁₁ NO ₂	117.15		Crystalline solid	[M+H-HCOOH]⁺ = 72 [M+H] ⁺ = 118 [2M+H-O] ⁺ = 219
	Leucine	C ₆ H ₁₃ NO ₂	131.17		Crystalline solid	[M+H]⁺ = 132 [2M+H] ⁺ = 263
D R U G S	Caffeine	C ₈ H ₁₀ N ₄ O ₂	194.19		Crystalline solid	[M+H]⁺ = 195
	Paracetamol	C ₈ H ₉ NO ₂	151.16		Crystalline solid	[M+H]⁺ = 152 [M+H-CO(CH ₃) ₂] ⁺ = 110

Table S1. A table describing the ions observed from positive ion mass spectrometry of selected volatiles and non-volatiles. It is important to note that the LTQ linear ion trap used for these experiments is limited to nominal mass resolution.

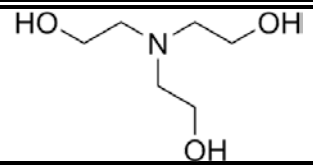
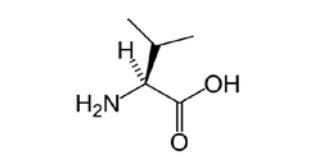
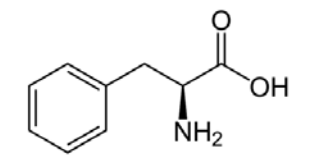
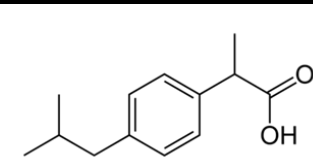
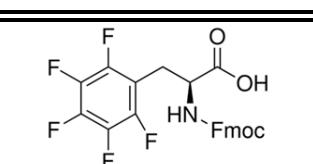
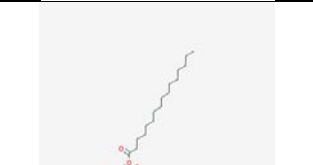
	Substance	Molecular formula	Mass, Da	Structure	Type of Substance	Negative ion mode (Dominant ion in bold)
P C P	Triethanol-amine	C ₆ H ₁₅ O ₃ N	149.11		Liquid	[2M-2(OH)-CH₂]⁻ = 250 [2M-2(OH)-CH ₂ +O] ⁻ = 266 etc.
	Valine	C ₅ H ₁₁ NO ₂	117.15		Crystalline solid	[M-H]⁻ = 116 [2M-H] ⁻ = 233
A M I N O A C I D S	Phenyl- alanine	C ₉ H ₁₁ NO ₂	165.19		Crystalline solid	[M-H]⁻ = 164
	Ibuprofen	C ₁₃ H ₁₈ O ₂	206.29		Crystalline solid	[M-H]⁻ = 205 [2M-H] ⁻ = 411
D R U G S	Fmoc	C ₂₄ H ₁₆ F ₅ NO ₄ (Fmoc - C ₁₅ H ₁₁ ClO ₂)	477.38		Crystalline solid	[M-H]⁻ = 476 [M+NO ₃] ⁻ = 539 [2M-H] ⁻ = 953
	PC(16:0/16:0) DPPC	C ₄₀ H ₈₀ NO ₈ P	734.04		Crystalline solid	[M+NO₃]⁻ = 795 [M-CH ₃] ⁻ = 718 [16:0 FA-H] ⁻ = 255

Table S2. A table describing the ions observed from negative ion mass spectrometry of selected volatiles and non-volatiles. It is important to note that the LTQ linear ion trap used for these experiments is limited to nominal mass resolution.

211113_micropadi_cardomonpos_1 #353 RT: 4.11 AV: 1 NL: 3.89E4
T: ITMS + p NSI Full ms [50.00-1000.00]

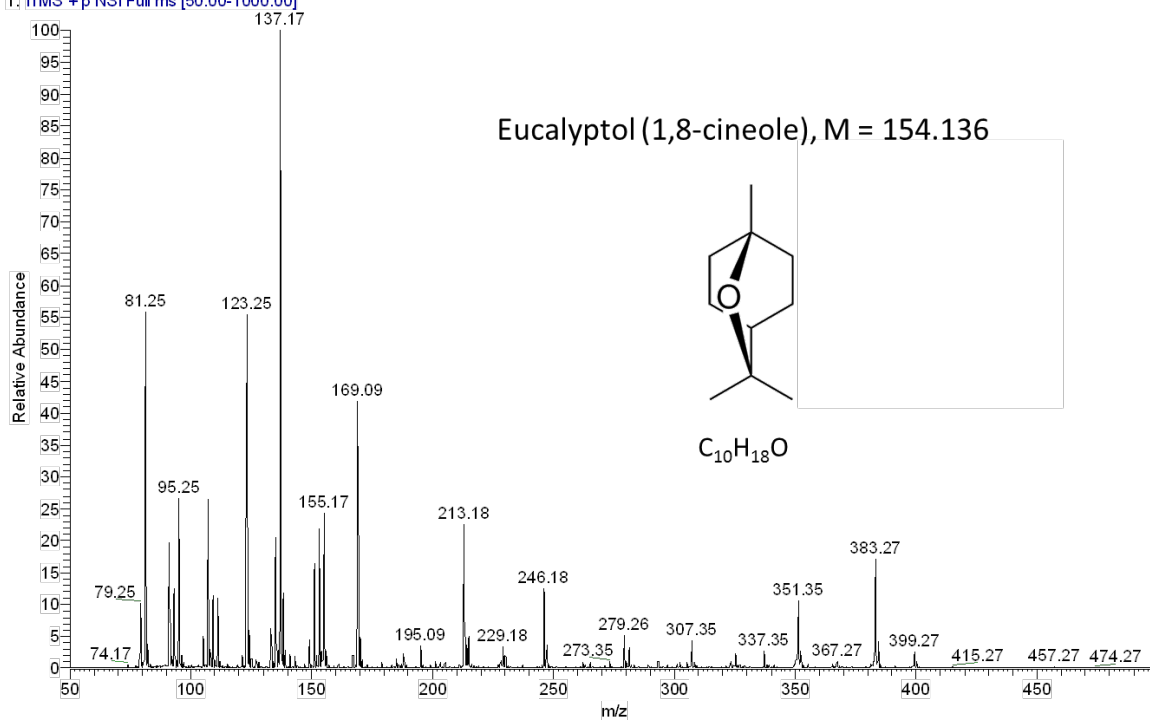


Figure S4. A typical positive ion mass spectrum recorded from a freshly cut cardamom seed produced using the LTQ linear ion trap, clearly showing the two ions used to construct the mass spectrometry images at m/z 81 (2.06×10^4 counts) and 95 (1.05×10^4 counts).

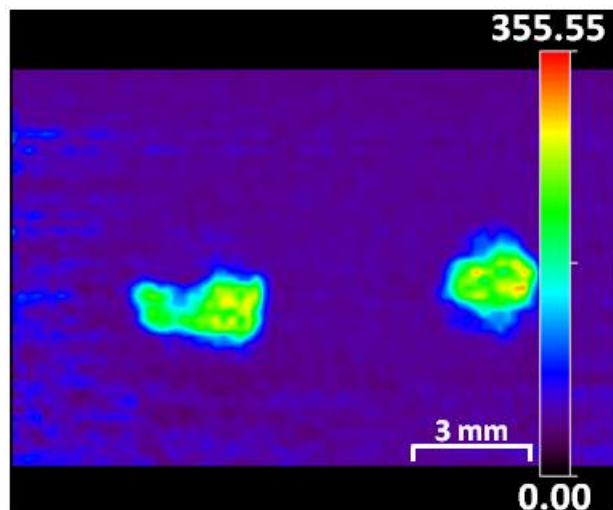


Figure S5. A positive ion MS image recorded from the freshly cut cardamom seeds using the variation in intensity (counts) of the ion located at m/z 95 as displayed by the scale bar on the right.

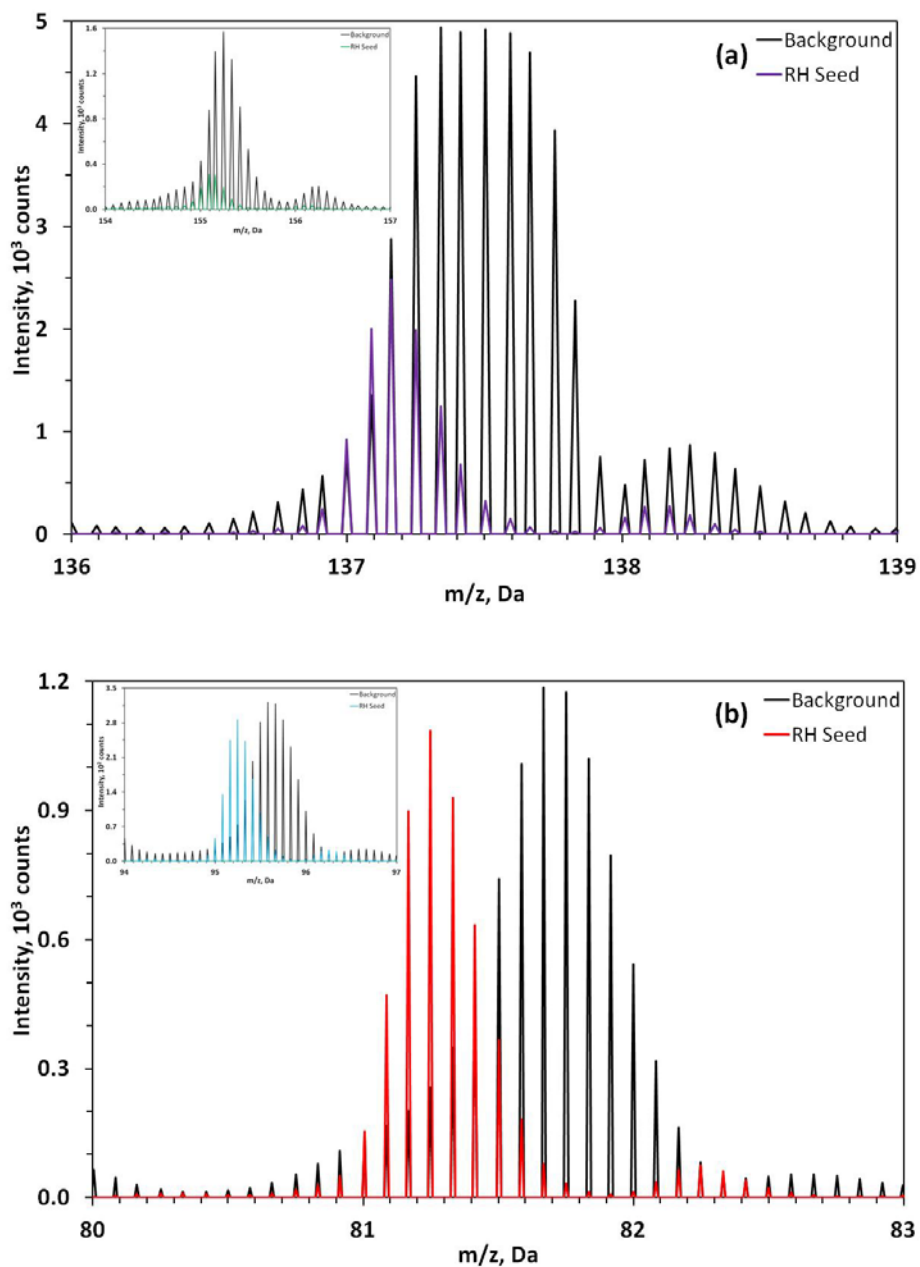


Figure S6. Positive ion mass spectra taken from both the right-hand seed and an ‘background’ area away from the seeds’ location contained within the region of the image for those ions located at m/z (a) 137 and 155 (inset) and (b) 81 and 95 (inset). The above spectra confirm that the ions located at m/z 81 and 95 are distinct ion series from those generated by plasma/air interactions as shown in (a), which are indistinguishable.