

**Fast Phenotyping of LFS- Silenced (Tearless) Onions by Desorption Electrospray
Ionization Mass Spectrometry (DESI-MS)**

Nigel I. Joyce,^{*†} Colin C. Eady,[†] Patrick Silcock,[#] Nigel B. Perry,[‡] and John W. van Klink^{*‡}

[†] The New Zealand Institute for Plant & Food Research Limited, Private Bag 4704,
Christchurch, New Zealand, [#]Department of Food Science, University of Otago, P.O. Box 56,
Dunedin, New Zealand, [‡] The New Zealand Institute for Plant & Food Research Limited,
Department of Chemistry, University of Otago, P.O. Box 56, Dunedin, New Zealand

Supporting Information:

Allium leaf analysis by DESI-MS summary of major precursor and product ions, Table S1;
DESI-MS average leaf precursor ion spectra, Figures S9–S18.

This material is available free of charge via the Internet at <http://pubs.acs.org>.

Table S1. *Allium* leaf analyses by DESI-MS

Leaf	MH ⁺ (MS ²) ^a
<i>A. cepa</i> (onion, cv. Pukekohe Longkeeper)	91 (73), 167 (73, 107, 125, 93, 59), 165 (73, 89, 105, 91)
<i>A. cepa</i> (onion - LFS- 05-J-0271)	91 (73), 113 , 163 (113, 145, 73), 165 (89, 73, 105, 113, 147)
<i>A. schoenoprasum</i> L. (Chive)	91 (73), 167 (73, 107, 125, 93, 59), 165 (73, 89, 105, 91) , 163 (113, 107, 145, 73)
<i>A. porrum</i> (leek)	91 (73), 167 (73, 107, 93, 125, 59), 165 (89, 73, 105, 113, 147), 163 (113, 107, 145, 101, 73)
<i>A. tuberosum</i> (Chinese chives)	99 , 111 (65, 69), 137 (73, 89, 95), 163 (121, 73, 107, 113)
<i>A. cepa</i> var. <i>aggregatum</i> (shallot)	91 (73), 198 (180, 163), 167 (73, 107, 125, 93, 59), 180 (163, 145), 145 (127, 99)
<i>A. cepa</i> var. <i>vivaparum</i> (Egyptian tree onion)	198 , 91 , 180 , 145 , 127 (no MS ² data collected)
<i>A. fistulosum</i> (spring onion)	91 (73), 167 (73, 107, 125, 93, 59), 165 (89, 73, 105, 91, 113), 151 (109, 123, 133)
<i>A. sativum</i> (garlic)	163 (121, 73, 91), 167 (73, 107, 125, 93, 59)
<i>A. ampeloprasum</i> (elephant garlic)	163 (121) (no MS ² data collected) ^b

^a Major precursor and product masses (averaged over a 3 min scan) listed in order from highest to lowest maximum abundance. (Some compounds reached high abundance over a short time frame but are comparably lower over an average period.)

^b MS² data absent but have presence of product *m/z* 121 from the in-source fragmentation of precursor *m/z* 163 as per garlic (compare with other precursor scans with sulfenic condensate only, in-source precursor *m/z* 163 - *m/z* 113).

Allium leaf Figures S9-S18

BG_D022-1009 #1-1485 RT: 0.01-3.00 AV: 1485 NL: 4.94E4
F: ITMS + c NSI Full ms [89.00-350.00]

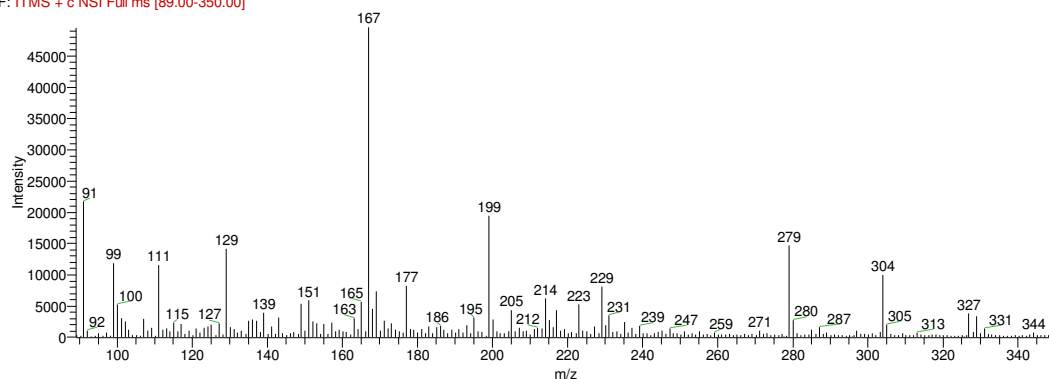


Figure S9 - *Allium cepa* (onion, cv. 'Pukekohe Longkeeper') – precursor scan average 0–3 minutes

D023-013ms2 #124-237 RT: 1.31-2.46 AV: 57 SB: 14 0.03-0.30 NL: 1.71E5
F: ITMS + c NSI Full ms [89.00-350.00]

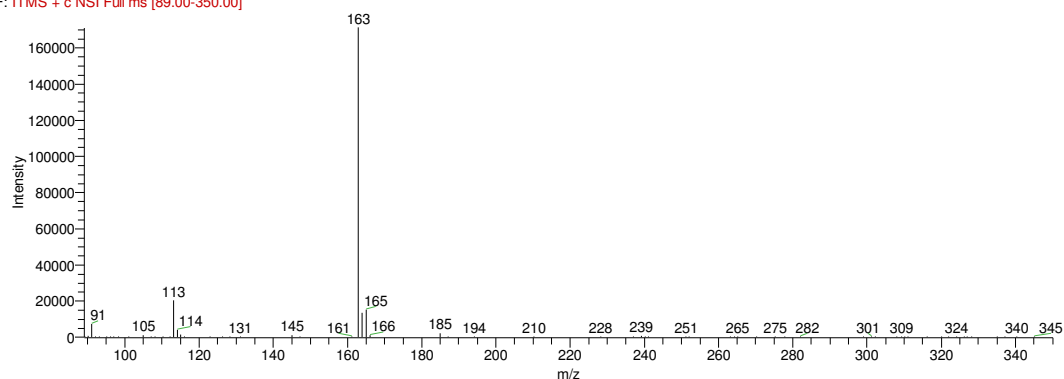


Figure S10 - LFS- Onion 05J0271 - precursor scan average 0–3 minutes

BG_D022-1004 #1-1398 RT: 0.01-3.00 AV: 1398 NL: 1.47E4
F: ITMS + c NSI Full ms [89.00-350.00]

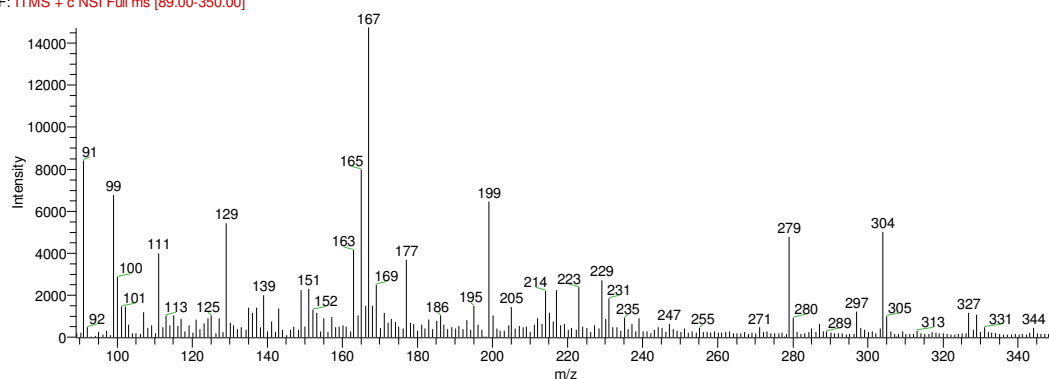


Figure S11 - *A. schoenoprasum* L. (chive) – precursor scan average 0–3 minutes

BG_D022-1036 #2-1492 RT: 0.01-3.00 AV: 1491 NL: 2.38E4
F: ITMS + c NSI Full ms [89.00-350.00]

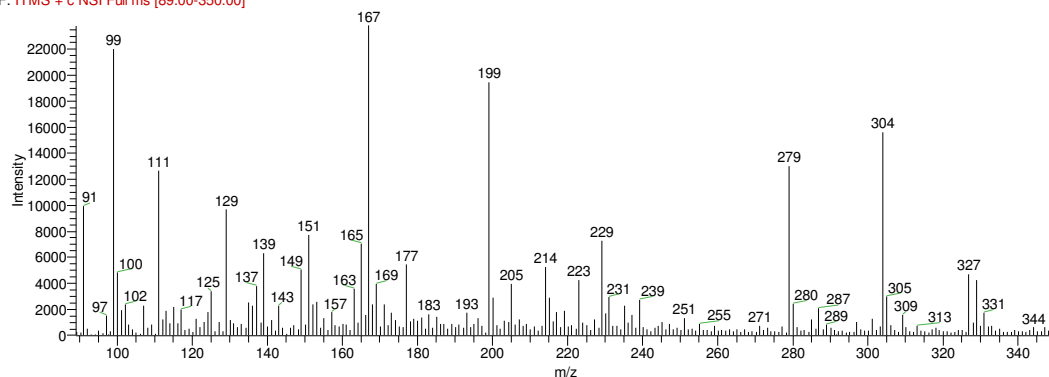


Figure S12 - *Allium porrum* (leek) - precursor scan average 0–3 minutes

BG_D022-1029 #1-1410 RT: 0.01-3.00 AV: 1410 NL: 3.72E4
F: ITMS + c NSI Full ms [89.00-350.00]

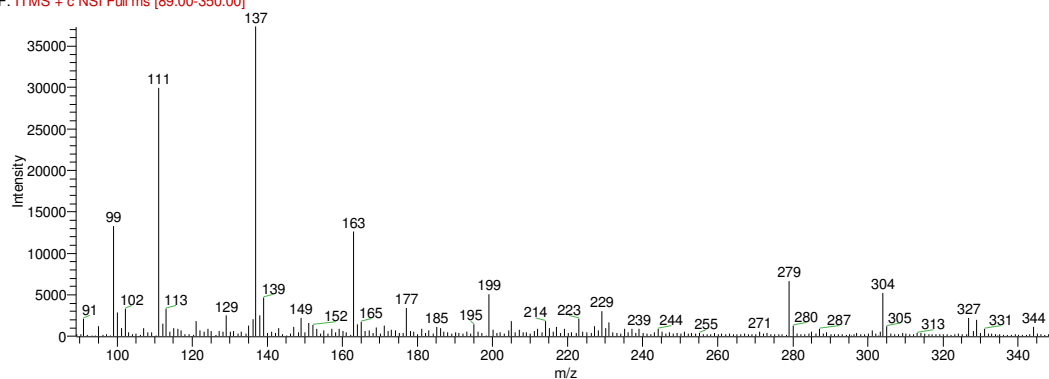


Figure S13 - *Allium tuberosum* (Chinese chives) - precursor scan average 0–3 minutes

BG_D022-1015 #1-1355 RT: 0.01-3.00 AV: 1355 NL: 2.98E4
F: ITMS + c NSI Full ms [89.00-350.00]

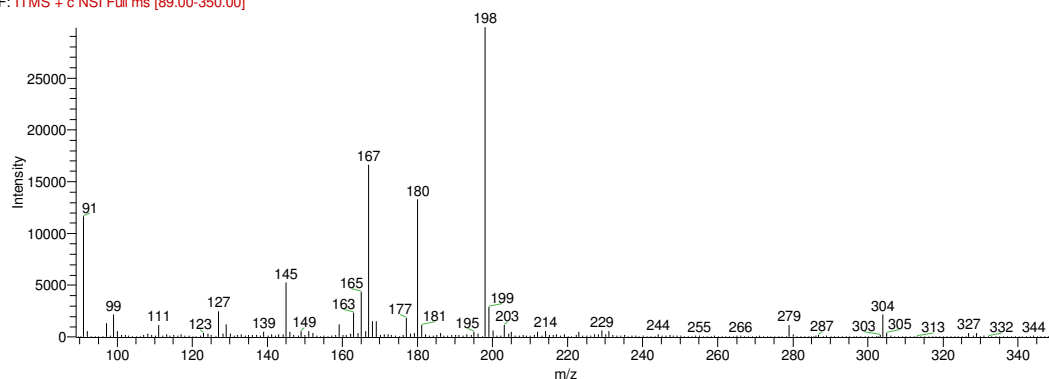


Figure S14 - *Allium cepa* var. *aggregatum* (shallot) – precursor scan average 0–3 minutes

BG_D022-1017 #2-1391 RT: 0.01-3.00 AV: 1390 NL: 5.45E4
F: ITMS + c NSI Full ms [89.00-350.00]

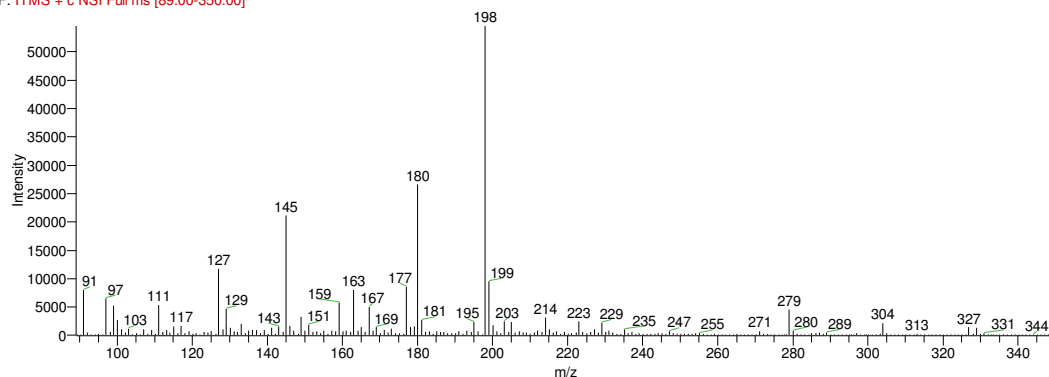


Figure S15 - *Allium cepa* var. *viviparum* (Egyptian tree onion) - precursor scan average 0–3 minutes

BG_D022-1020 #1-1400 RT: 0.01-3.00 AV: 1400 NL: 9.70E4
F: ITMS + c NSI Full ms [89.00-350.00]

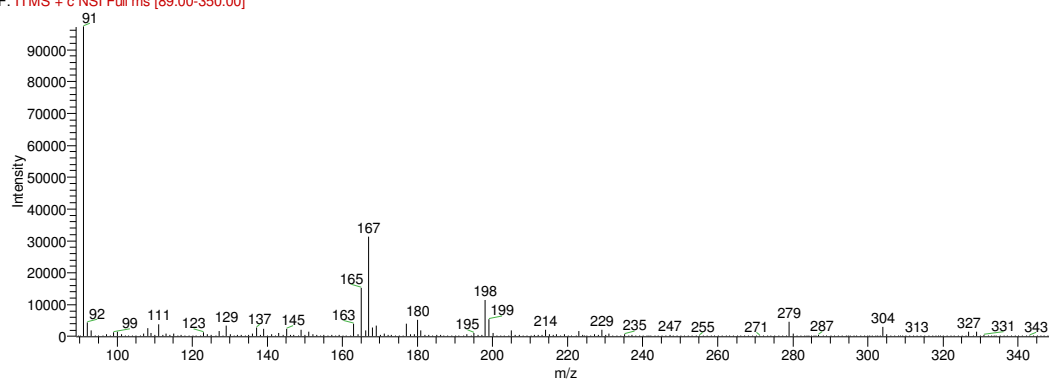


Figure S16 - *Allium fistulosum* (spring onion) - precursor scan average 0–3 minutes

BG_D022-1011 #2-1499 RT: 0.01-3.00 AV: 1498 NL: 5.73E4
F: ITMS + c NSI Full ms [89.00-350.00]

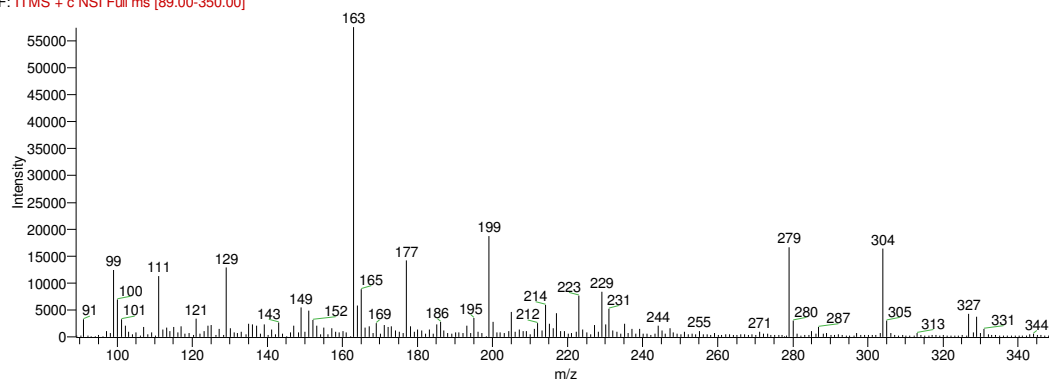


Figure S17 - *Allium sativum* (garlic) - precursor scan average 0–3 minutes

BG_D022-1026 #1-1421 RT: 0.01-3.00 AV: 1421 NL: 1.01E5
F: ITMS + c NSI Full ms [89.00-350.00]

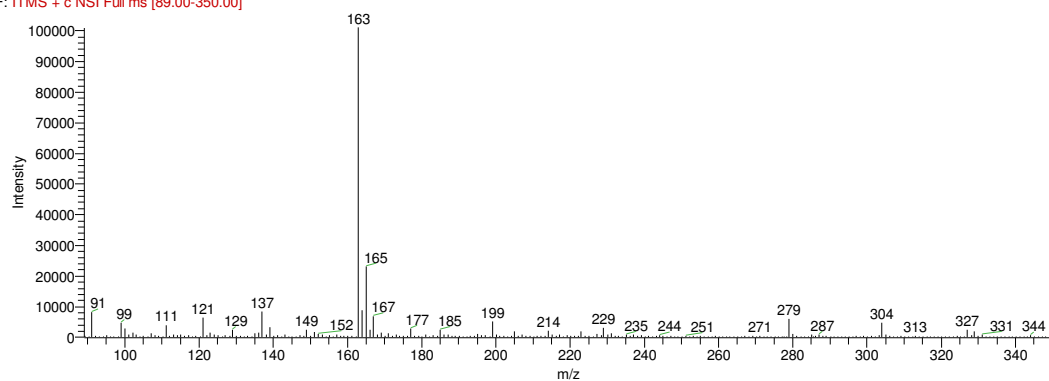


Figure S18 - *Allium ampeloprasum* (elephant garlic) - precursor scan average 0–3 minutes

END