

Supplementary Materials For:

Quantitative Analysis of NDMA in Drug Products: A Proposed High-Throughput Approach Using Headspace-SIFT-MS

Mark J. Perkins¹, Colin J. Hastie¹, and Vaughan S. Langford^{2,*}

1. Element Lab Solutions, Cambridge CB3 0NA, United Kingdom

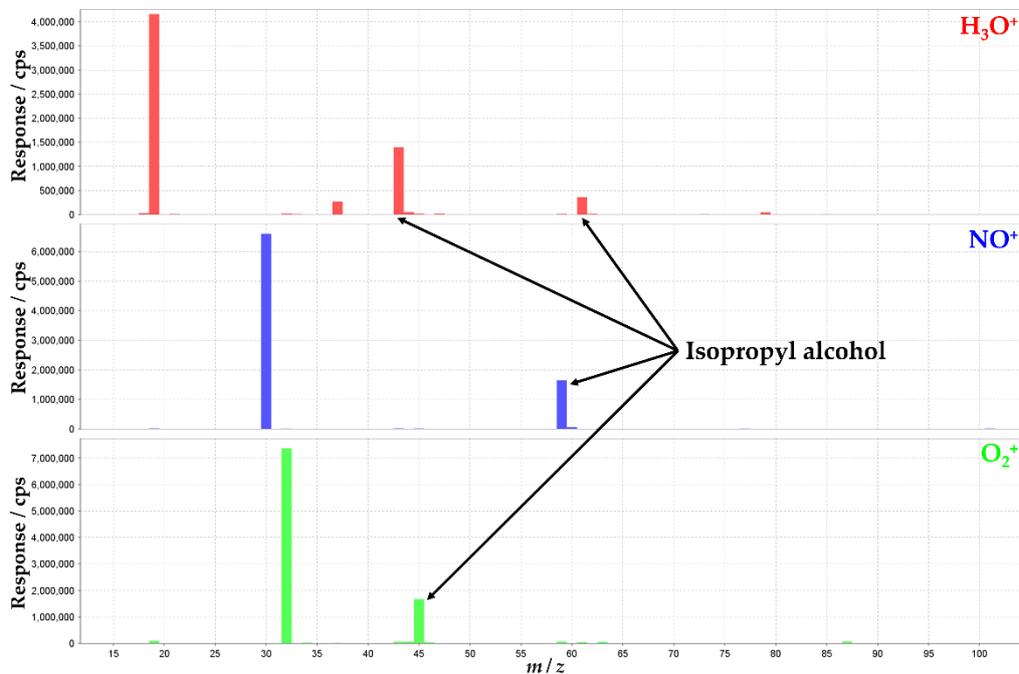
2. Syft Technologies Limited, Christchurch 8011, New Zealand

Table of Contents

Figure S1. SIFT-MS full-scan mass spectra of the two ranitidine-containing drug products containing relatively high levels of residual solvents.	Page 2
Figure S2. NDMA response in presence of (a) methanol and (b) 50:50 methanol:acetone mix.	Page 3
Figure S3. Repeatability of triplicate MHE-SIFT-MS measurements of NDMA (using $\text{NO}^+ 74$) in 300-mg samples of the ranitidine drug products.	Page 3
Figure S4. MHE-SIFT-MS results (natural logarithm of headspace concentration as function of injection number) for NDMA in the valsartan-containing drug product.	Page 4

Figure S1. SIFT-MS full-scan mass spectra of the two ranitidine-containing drug products containing relatively high levels of residual solvents (a) isopropyl alcohol in sample R1 and (b) ethanol in sample R2. The largest spectral features peaks are from the reagent ions, H_3O^+ (m/z 19), NO^+ (30), and O_2^{+*} (32).

(a) R1



(b) R2

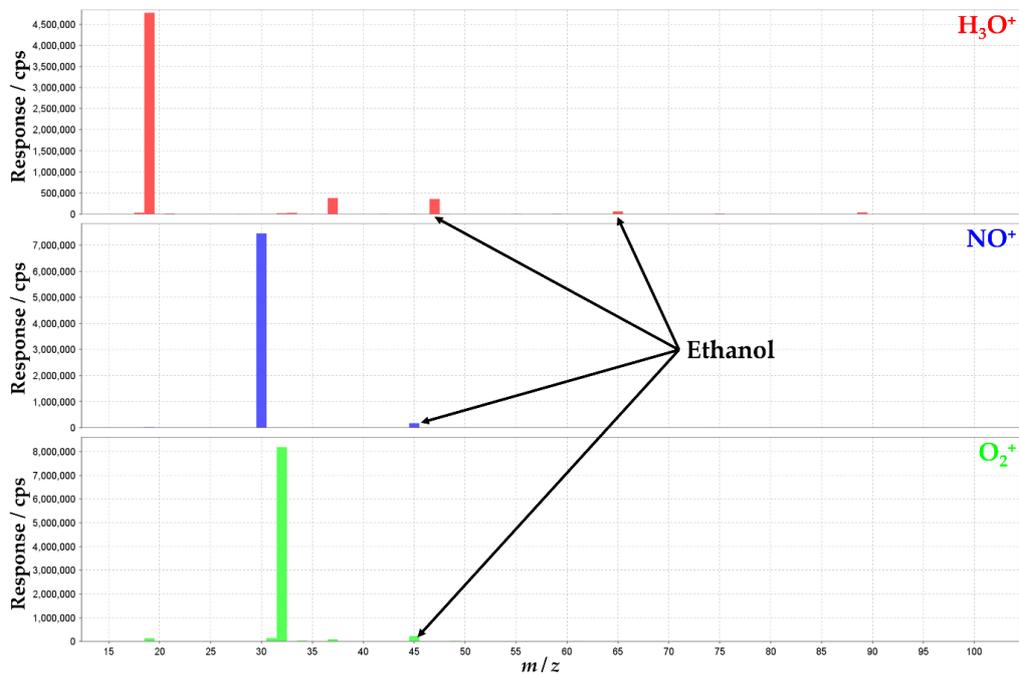


Figure S2. NDMA response in presence of (a) methanol and (b) 50:50 methanol:acetone mix. See Section 2.2.2 of the main article for details on how these curves were created.

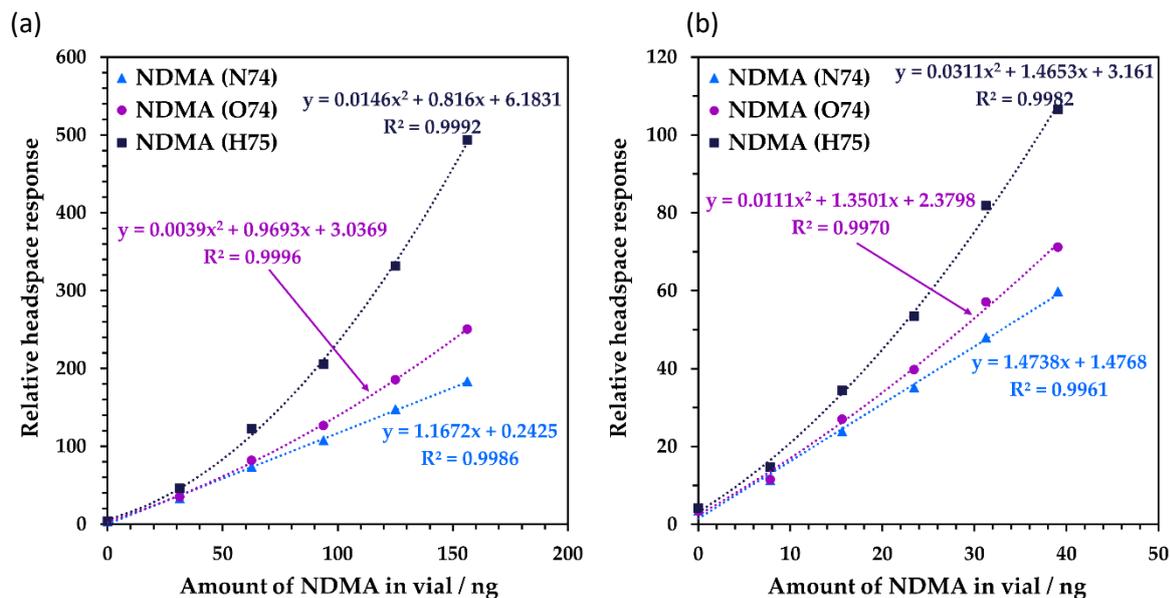


Figure S3. Repeatability of triplicate MHE-SIFT-MS measurements of NDMA (using NO^+ 74) in 300-mg samples of the ranitidine drug products (a) R1 and (b) R2.

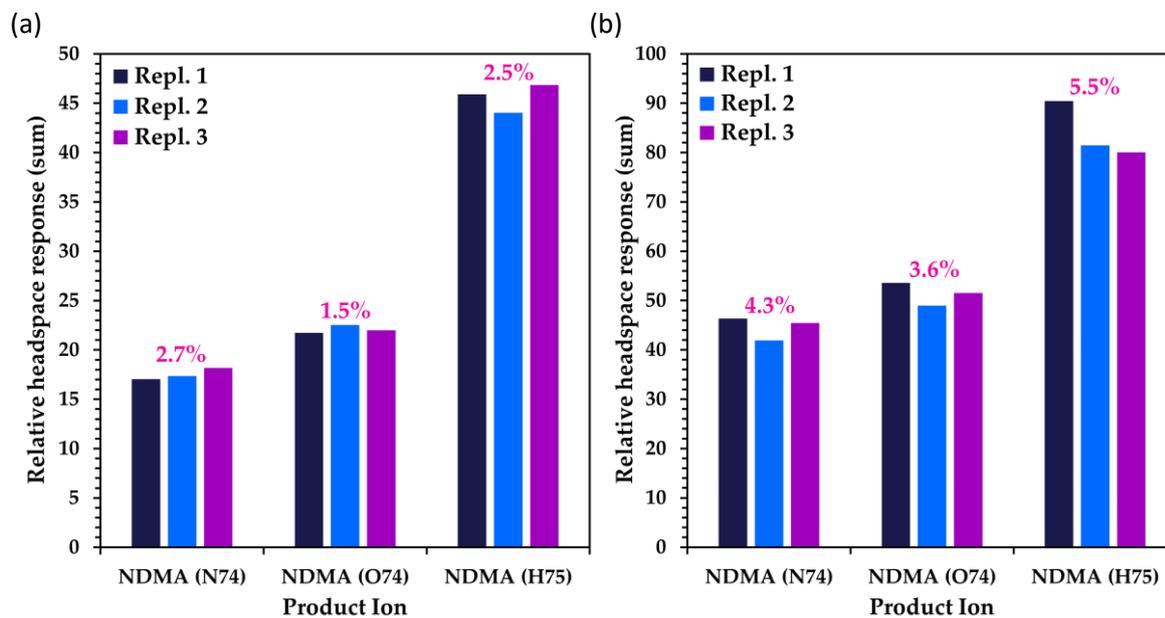


Figure S4. MHE-SIFT-MS results (natural logarithm of headspace concentration as function of injection number) for NDMA in the valsartan-containing drug product. Results for quantification and qualifier ions are shown. Note that the quantitation at this point is based on the SIFT-MS library data; calibration is applied subsequently.

