

## Exploring the potential of NTME/GC-MS, in the establishment of urinary volatonic profiles. Lung cancer patients as case study

Priscilla Porto-Figueira<sup>a</sup>, Jorge Pereira<sup>a</sup>, Wolfram Miekisch<sup>b</sup>, José S. Câmara<sup>a,c,\*</sup>

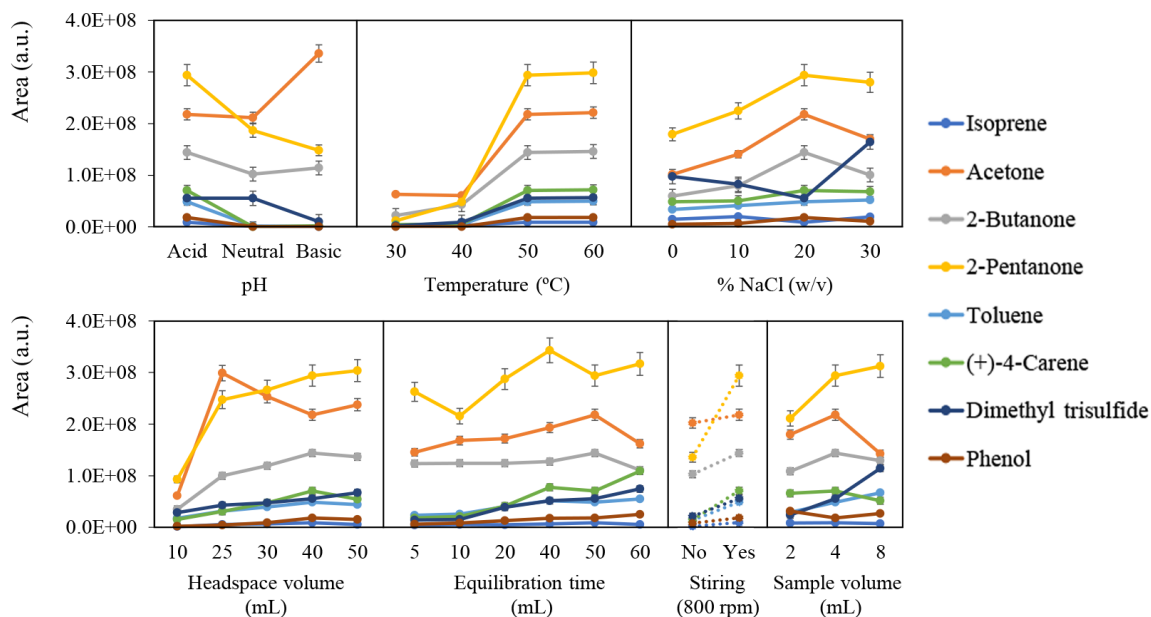
<sup>a</sup> CQM-UMa, Centro de Química da Madeira, Universidade da Madeira, Campus Universitário da Penteada, 9020-105 Funchal, Portugal;

<sup>b</sup> Department of Anaesthesiology and Intensive Care Medicine, Rostock Medical Breath Research Analytics and Technologies (ROMBAT), University Medicine Rostock, Rostock, Germany.

<sup>c</sup> Faculdade de Ciências Exatas e da Engenharia da Universidade da Madeira, Campus Universitário da Penteada, 9020-105 Funchal, Portugal

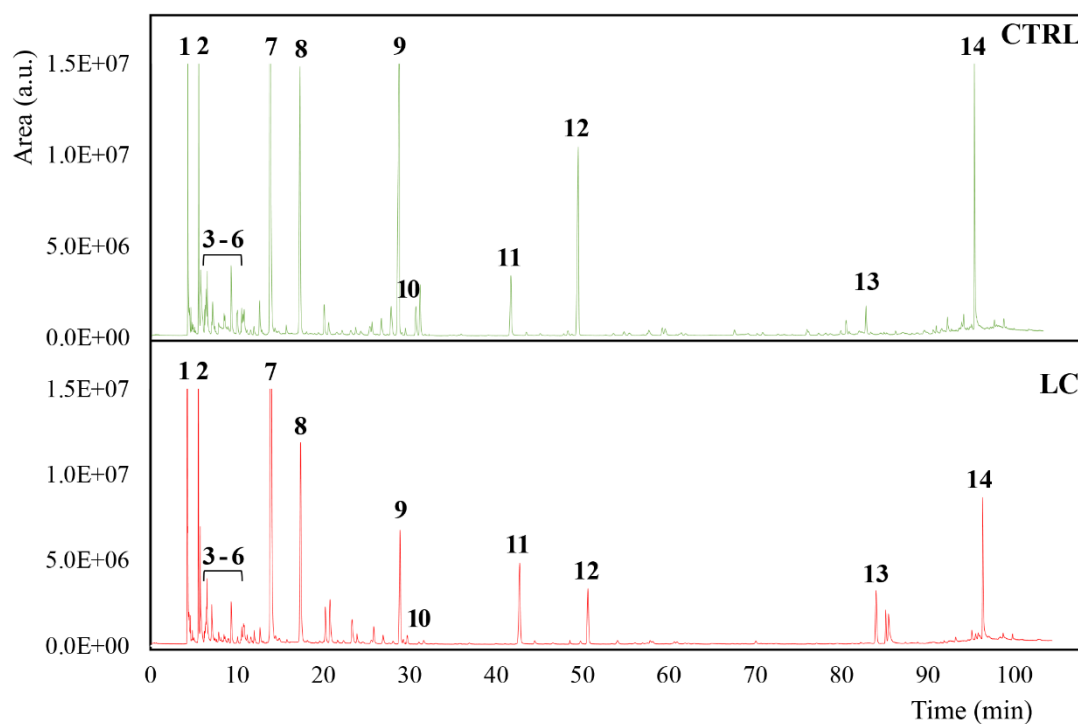
### Supplementary Figures

#### Supplementary Fig. 1



Supplementary Fig. 1: Optimization of different parameters affecting NTME (pH, extraction temperature, ionic strength through NaCl concentration, volume of the sample headspace, equilibration time, sample stirring and volume) by selected VOMs.

## Supplementary Fig. 2



Supplementary Fig. 2: Typical chromatograms obtained with control (CTRL) and lung cancer (LC) urine samples. Legend: 1 – Furan, 2 – Acetone, 3 - Tetrahydro-2,2,5,5-tetramethylfuran, 4 - 2-Butanone, 5 - 2-Pentanone, 6 - 2,4-Dimethyl-3-pentanone, 7 - Dimethyl disulphide, 8 - 4-Heptanone, 9 - o-Cymene, 10 - methyl allyl disulphide, 11 - Dimethyl trisulfide, 12 - p-cymenene, 13 - Dehydro-Ar-ionene, 14 - p-Cresol