

## OT6 Ion-molecule reactions for medical diagnostics

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Mass overlaps from CI of patient's breath using SIFT-MS can be resolved by heat.

Selected ion flow tube mass spectrometry provides real time quantitative information on breath metabolites. Because of the high water content of human breath, water molecules cluster to ions formed from common breath volatiles (ammonia, acetone, ethanol and acetic acid) with multiple water molecule clusters being formed at times. These cluster ions result from ion-molecule association processes and are usually weakly bound. Chloramines ( $H_xNCl_y$ ) and bromamines ( $H_xNBr_y$ ) are by-products of neutrophils and eosinophils and are thought to be present in the airways of individuals with respiratory disease. These haloamines may therefore act as biomarkers for people with respiratory inflammation. Chemical ionization (CI) of the haloamines form ion products that are isobaric with water cluster ions of common breath volatiles. We present data showing how isobaric overlaps of the product ions arising from chemical ionization reactions of haloamines and those of water cluster ions of volatiles in flow tubes can be eliminated by heating the flow tube.

Water cluster ions of breath volatiles are formed as termolecular reactions in a flow tube. Using acetone as an example with  $H_3O^+$  as the chemical ionization reagent, the following products may be formed:  $CH_3COCH_3 \cdot H^+$  (m/z 59),  $CH_3COCH_3 \cdot H^+ \cdot H_2O$  (m/z 77),  $CH_3COCH_3 \cdot H^+ \cdot (H_2O)_2$  (m/z 95).