

Supporting Information

Time-resolved Thermal Desorption Miniature Ion Trap Mass Spectrometry for Rapid and Simultaneous Quantification of Multiple Cooling Agents in Complex Matrices

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S-1. Structural formulas of four cooling agents.

Structural formulas of four cooling agents (WS-3, WS-5, Evercool 180, OW22Q34GIJ) are shown in Fig. S1.

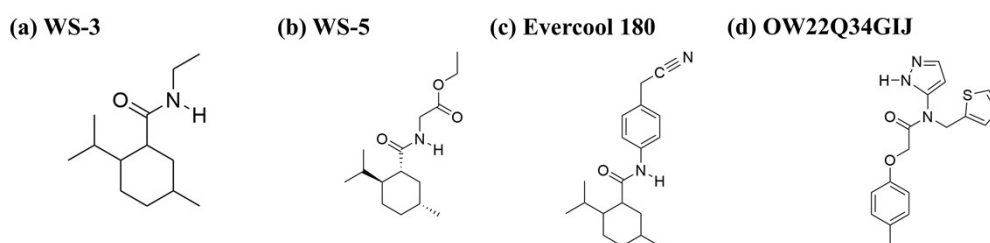
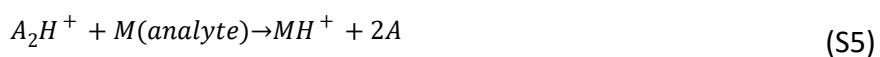
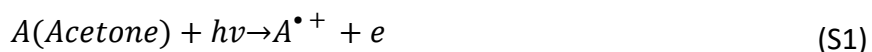


Fig. S1. Structural formulas of four cooling agents (a) WS-3; (b) WS-5; (c) Evercool 180; (d) OW22Q34GIJ.

S-2. Mechanism of temperature-induced changes in signal strength of acetone dimer ions.

The product ions MH^+ are generated through a proton transfer reaction between the acetone dimer ions A_2H^+ and the analyte M. When the concentration of analytes with high proton affinity is high, the ionization of analyte with low proton affinity will be inhibited, as shown in Fig. 3 and Fig. 4. One potential solution is to increase the concentration of reagent ions A_2H^+ , which are produced by the following reactions:



Thus, the concentration of reagent ions can be enhanced by increasing the evaporation temperature of acetone, which can be accomplished. As shown in Fig. S2, the signal intensity of the reagent ions increased by a factor of two with rising temperature as the evaporation temperature from room temperature to 40 °C.

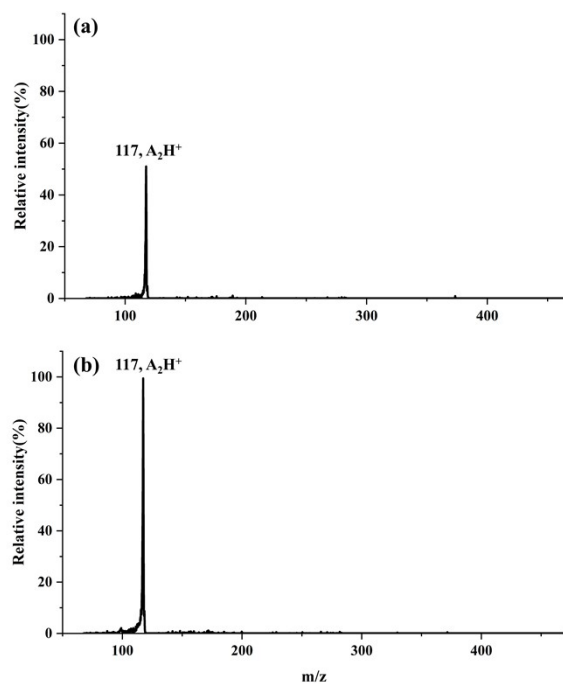


Fig. S2. Mass spectra of acetone dimer ions at different evaporation temperature (a) room temperature and (b) 40 °C.