

**Infrared Atmospheric Solids Analysis Probe (IR-ASAP) Mass Spectrometry for
Ambient Analysis of Volatile Compounds without Heated Gas**

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Supplemental Table 1, Scheme 1, and Figures S1-S7

Table S1: Instrumentation setting of ASAP and IR-ASAP.

Settings	ASAP	IR-ASAP
Sheath gas flow rate	2 psi	-
Aux gas flow rate	8 psi	-
Spray voltage	3.5 kV	2.5-3.0 kV
Capillary temp.	300 °C	300 °C
Capillary voltage	25.0 V	25.0 V
Tube lens voltage	65.0 V	65.0 V
Skimmer voltage	14.0	14.0 V
Heater temp.	250 °C	-

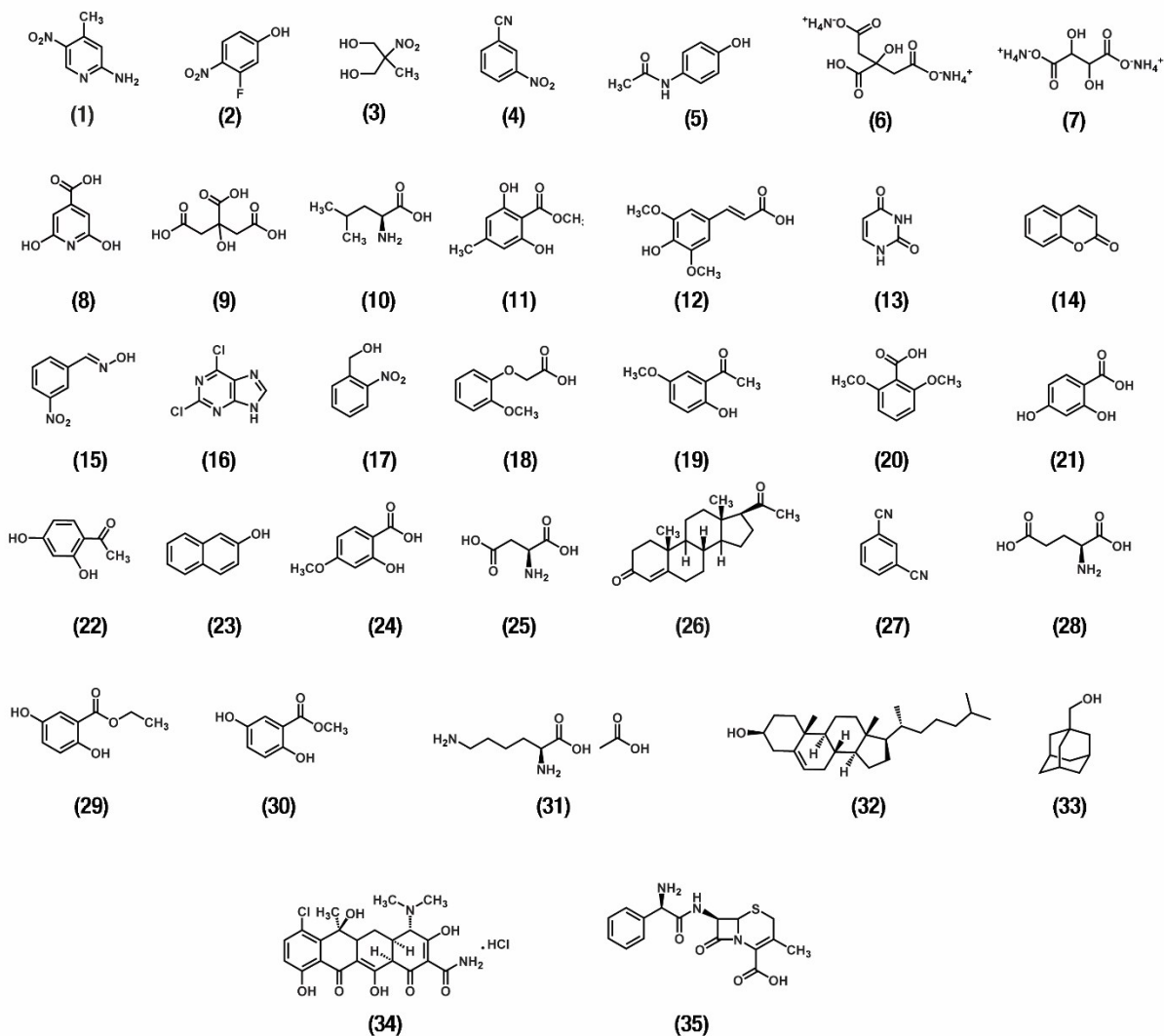
Scheme S1: Compounds used in this study

Figure S1: Mass spectrum of sinapinic acid (MW 224.21) using (a)ASAP, and (b) IR-ASAP.

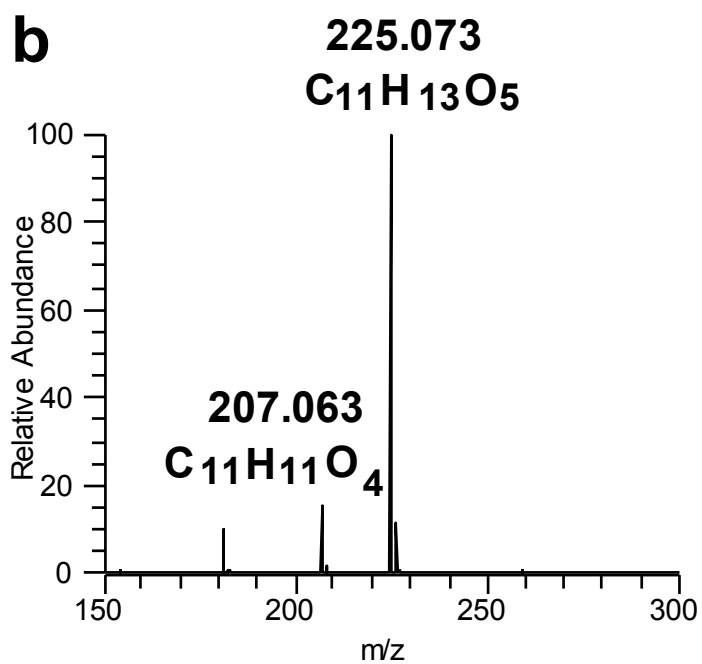
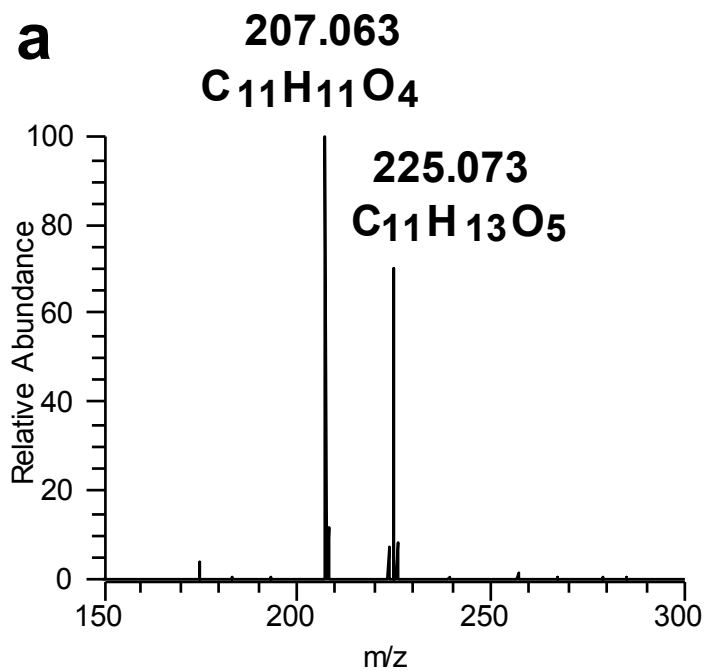


Figure S2: Mass spectrum of citrazinic acid (MW 155.11) using (a)ASAP, and (b) IR-ASAP.

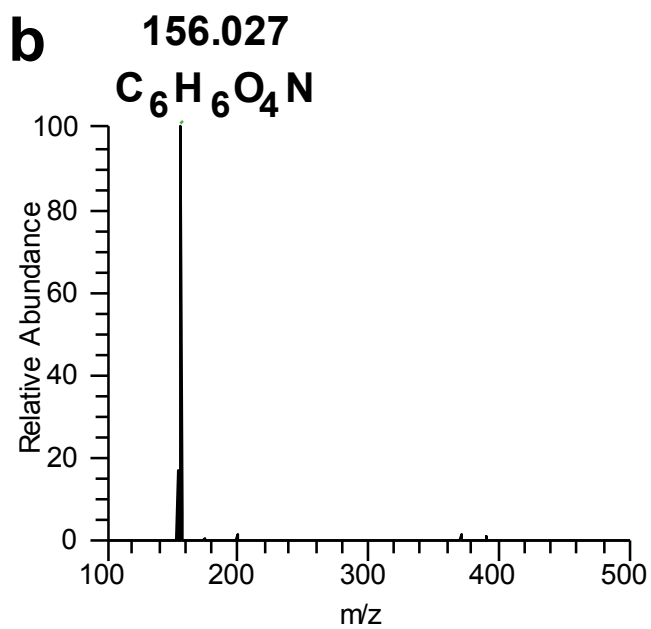
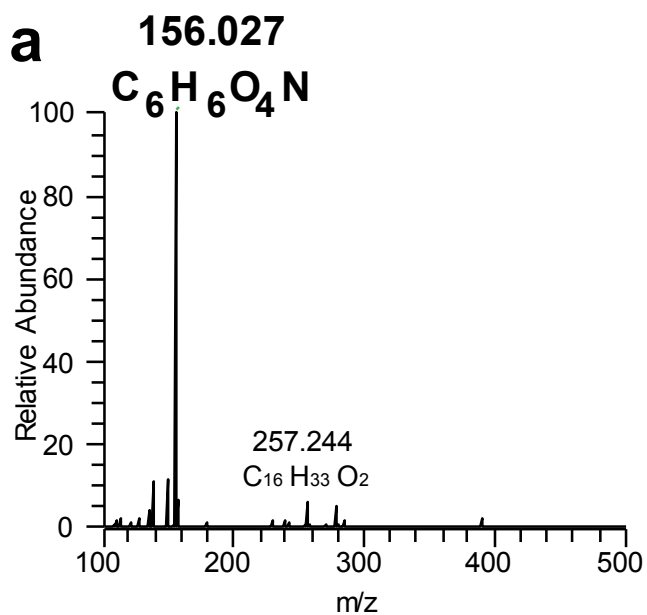


Figure S3: Mass spectrum of L-aspartic acid (MW 133.10) using (a)ASAP, and (b) IR-ASAP.

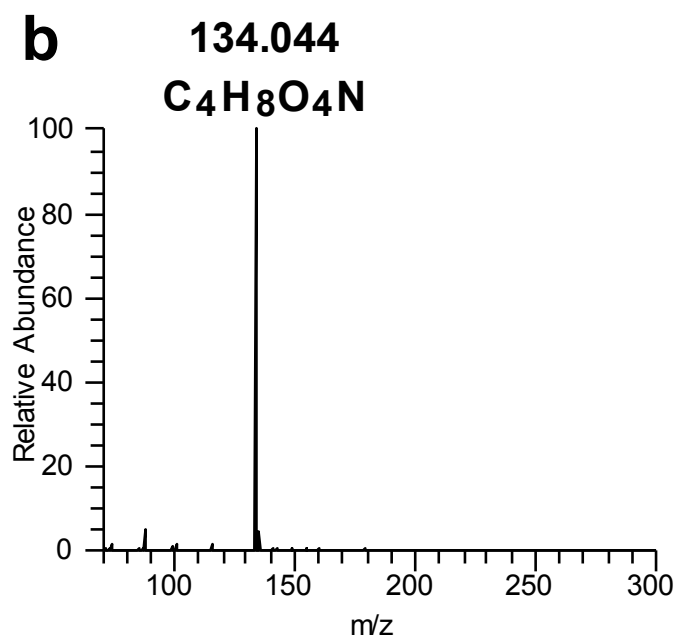
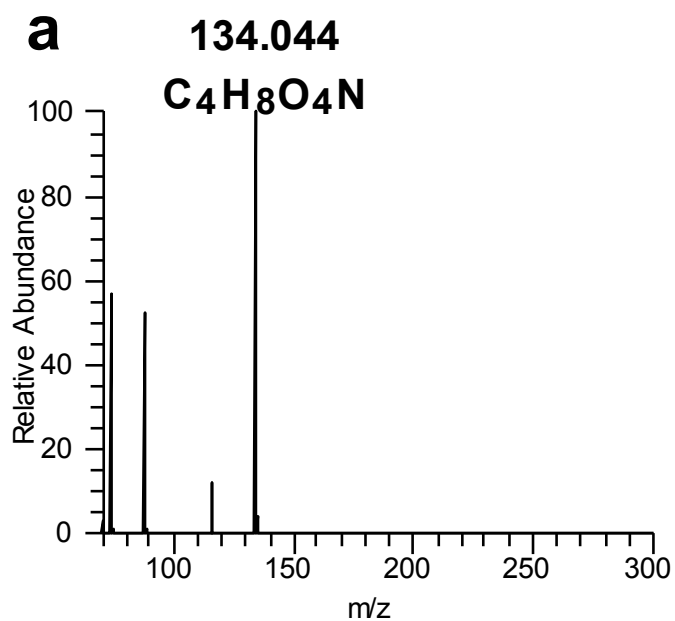


Figure S4: Mass spectrum of 2-amino-4-methyl-5-nitropyridine (MW 153) using (a) ASAP and (b) IR-ASAP.

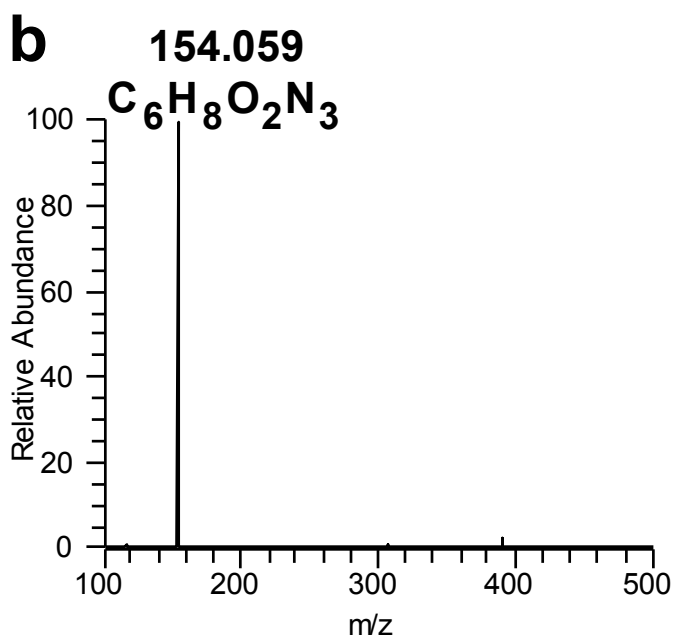
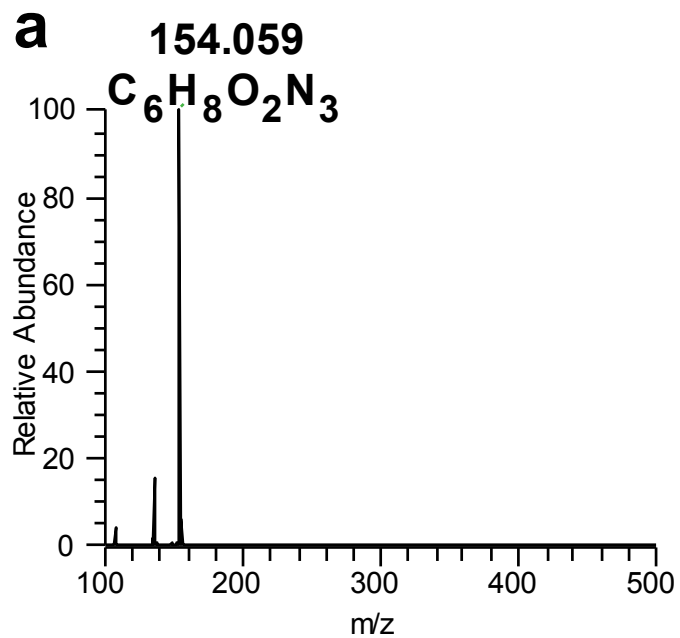


Figure S5: Mass spectrum of acetaminophen (MW 151.17) using (a)ASAP, and (b) IR-ASAP.

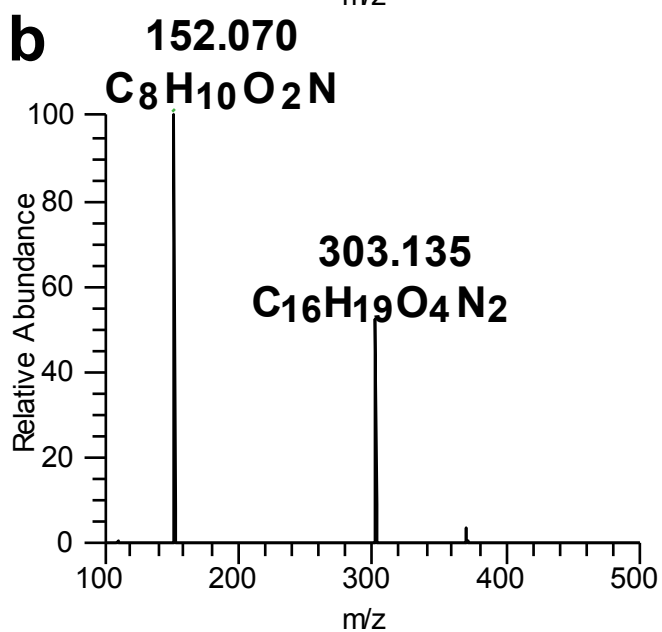
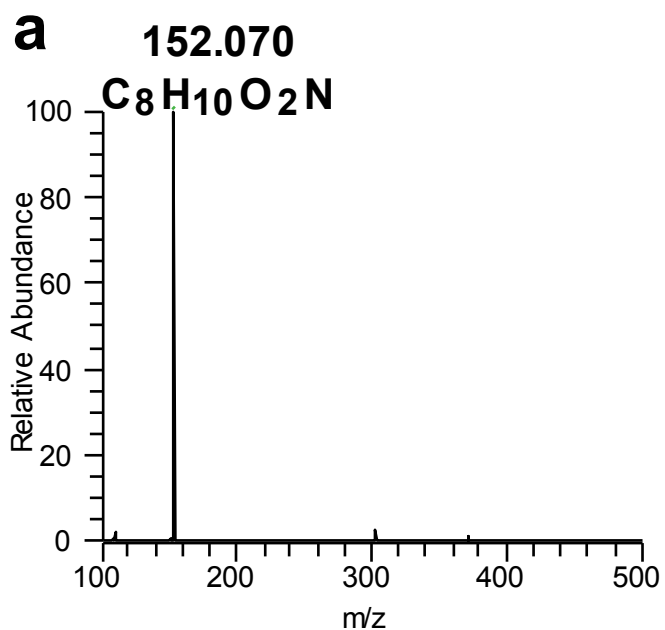


Figure S6: Mixture of amino acids acquired by IR-ASAP. Amounts loaded on melting point tube was 100 pm for gly (1.0e6), ala (2.9e6), pro (6.0e6), val (5.7e6), arg (ND), thr (3.4e6), lys (2.1e6), and gln (2.5e5), 50 pm for ser (8.9e5), leu/ile (7.4e6), met (1.7e6), his (6.0e4), phe (3.8e6), tyr (7.1e5), asn (3.4e5), asp (1.8e3), glu (6.3e3), orn (6.1e5), and cit (7e3), and 25 pm for trp (2.2e5). Ion abundances are given in parenthesis.

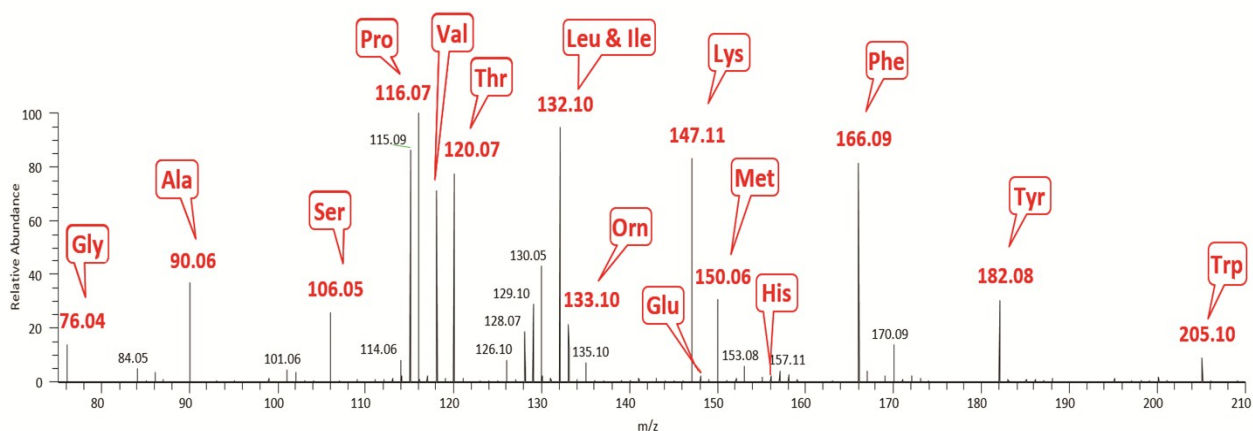


Figure S7: IR-ASAP of 5 ppm solution of acetaminophen (MW 152.071) on an Orbitrap Exactive. Top spectrum is from 1 μ L of this solution spotted on a melting point tube and bottom spectrum is spiked synthetic urine at the same concentration with 1 μ L added to the melting point tube. Insets show m/z range 151.5 to 153.5.

