Electronic Supplementary Material (ESI) for Sensors & Diagnostics.

Supplementary Information

Device operation procedure

The experimental procedure to complete a test with the device begins by pressing the 'start measurement' button on the HDMI touchscreen. Upon pressing the button, the device counts three seconds for the user to get ready to exhale, and then displays a 20-second countdown during which the user exhales continuously into the sterile mouthpiece. After the exhalation, the device analyzes the breath. Once the analysis is complete (i.e., after 10 minutes), the device goes back to the initial screen with the button 'start measurement'. At all times, the measurement can be interrupted by pressing the 'cancel' button.

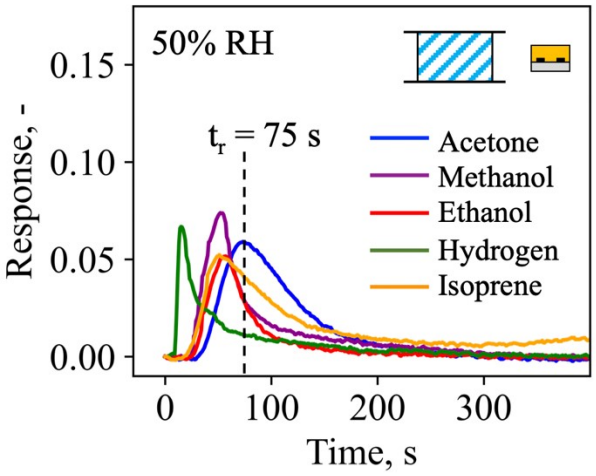

Figure S1: Sensor response to 30 s exposure of the analytes acetone (blue), methanol (purple), ethanol (red), hydrogen (green), and isoprene (orange), each 1 ppm as single analytes, with only the separation column ahead of the sensor. The acetone retention time (t_r) is indicated with a dashed line.

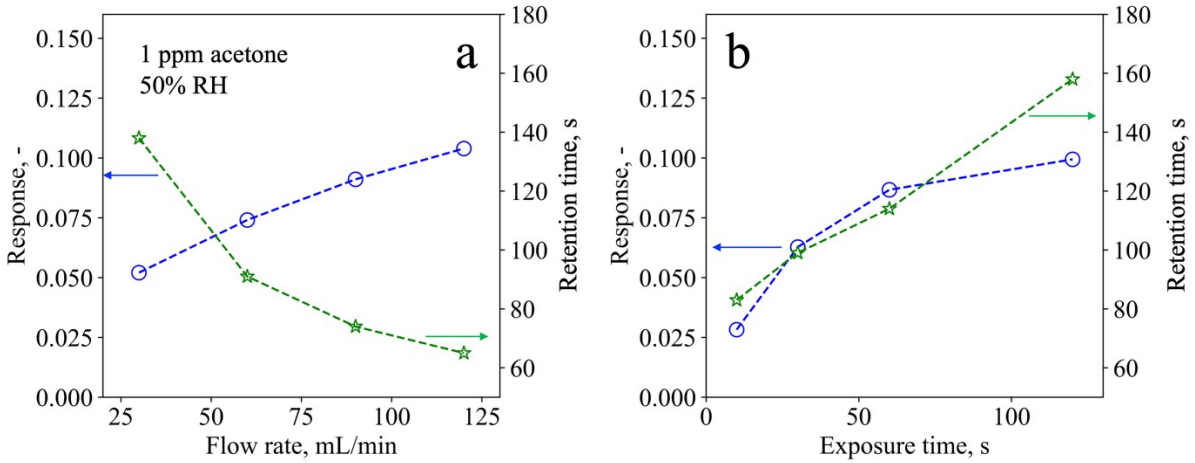

Figure S2: Device response (circle) and retention time (stars) to 1 ppm acetone at 50% RH as a function of flow rate **(a)** and exposure time **(b)**.

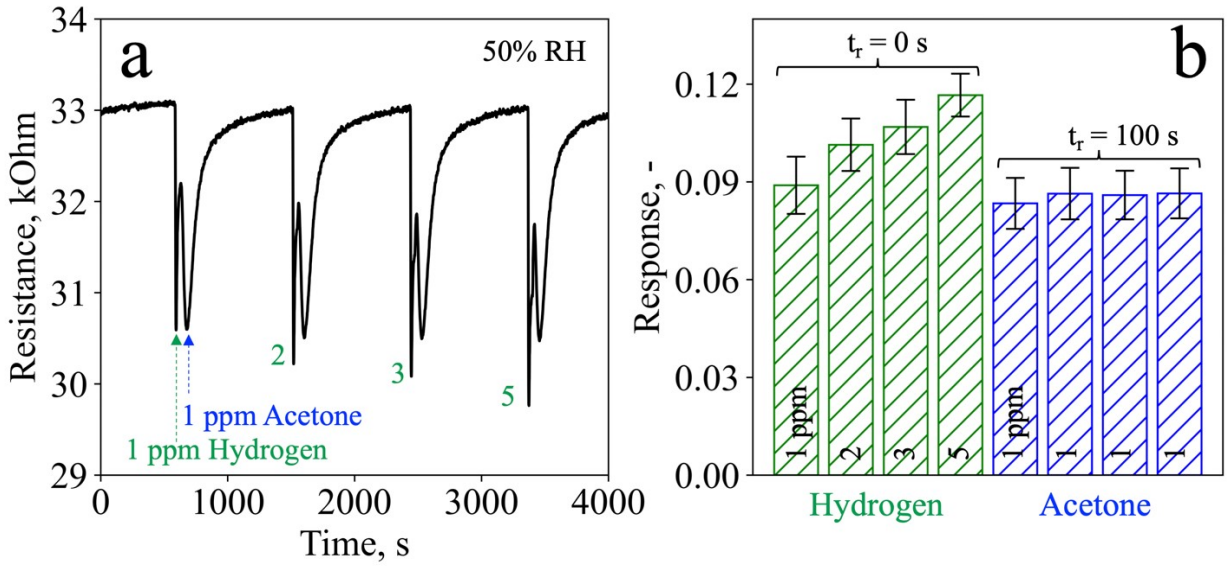

Figure S3: (a) Device resistance upon exposure to 1 ppm acetone together with 1, 2, 3, and 5 ppm hydrogen at 50% RH. **(b)** Corresponding device response for 1, 2, 3, and 5 ppm hydrogen (green, determined at t_r = 0 s) and acetone (blue, t_r = 100 s). Note that this device may be used also for the detection of hydrogen. As expected, the acetone response is hardly affected by varying hydrogen concentrations. Error bars represent the standard deviation of three separate detectors.

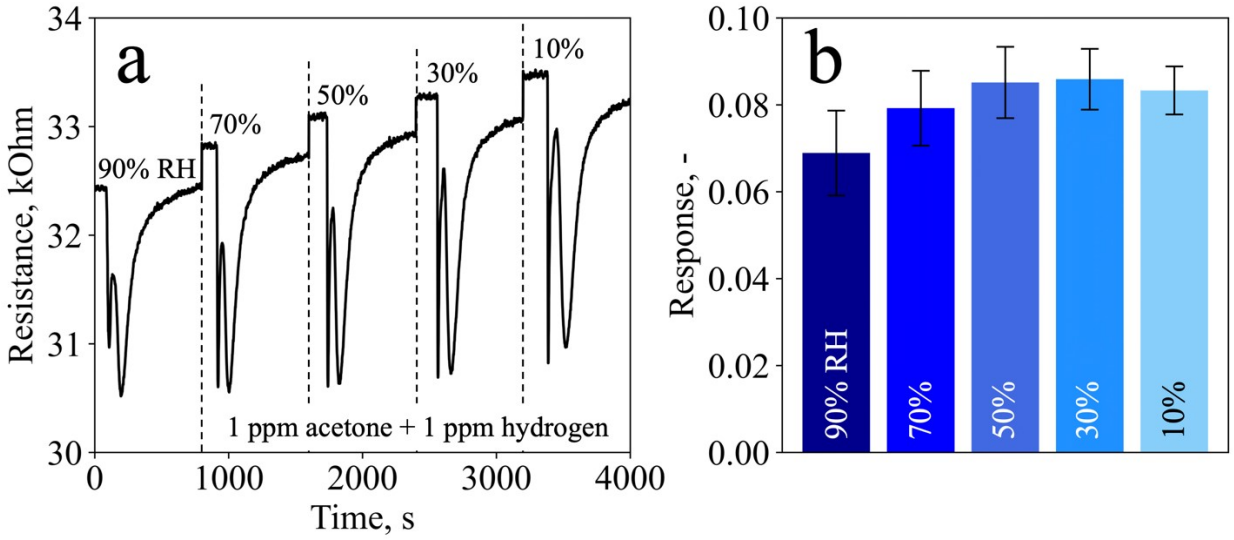

Figure S4: (a) Device resistance upon exposure to 1 ppm acetone together with 1 ppm hydrogen at 90, 70, 50, 30, and 10% RH. **(b)** Corresponding device response for 1 ppm acetone as a function of RH. The error bars represent the standard deviation of three separate detectors.

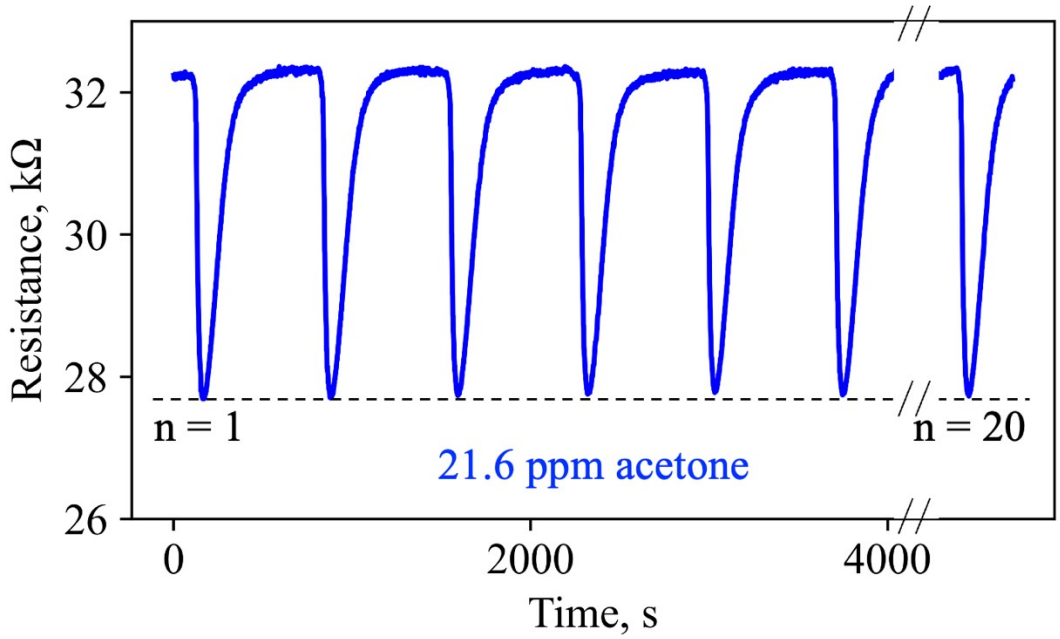

Figure S5: Raw data of the device when measuring the highest calibration standard containing 21.6 ppm acetone for N = 20 cycles.

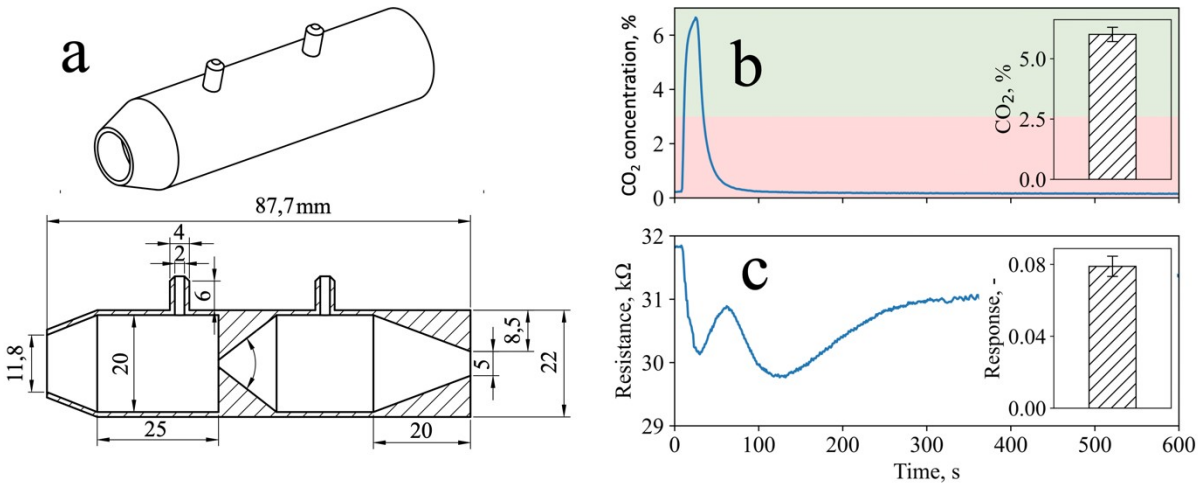

Figure S6: (a) Schematic of the sampling unit, together with a sketch showing the sampling unit dimensions. **(b)** CO_2 concentration measured during a breath exhalation. End-tidal concentrations (above 3%) are indicated in green, and the inset shows the error bar for three identically produced sampling units. **(c)** Corresponding device resistance, with the sensor response and error bar of three sampling units as an inset.

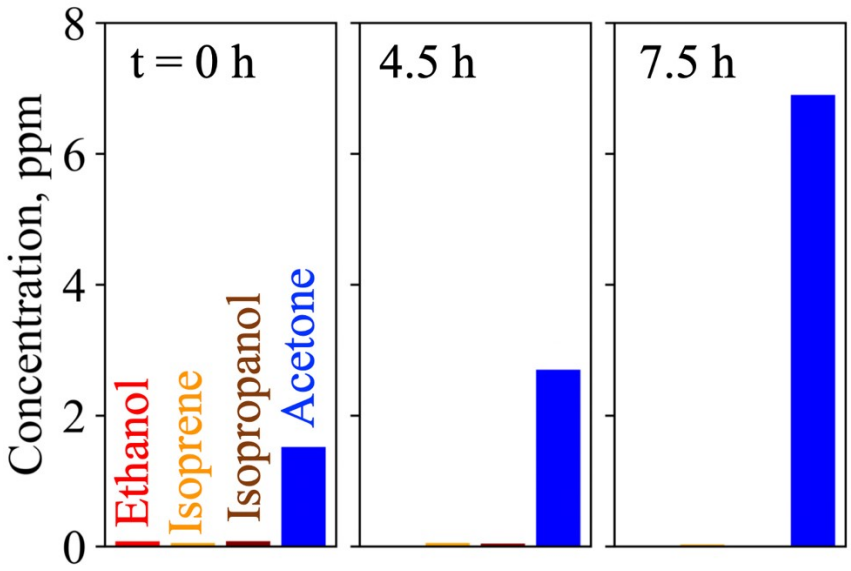

Figure S7: PTR-ToF-MS measured concentrations of ethanol (red), isoprene (orange), isopropanol (brown), and acetone (blue) for three exhalations of volunteer #1 at t = 0 h (at 8:00), 4.5 h and 7.5 h of the ketogenic diet. The concentrations were determined at the acetone peak concentration at t = 125 s of each breath exhalation.

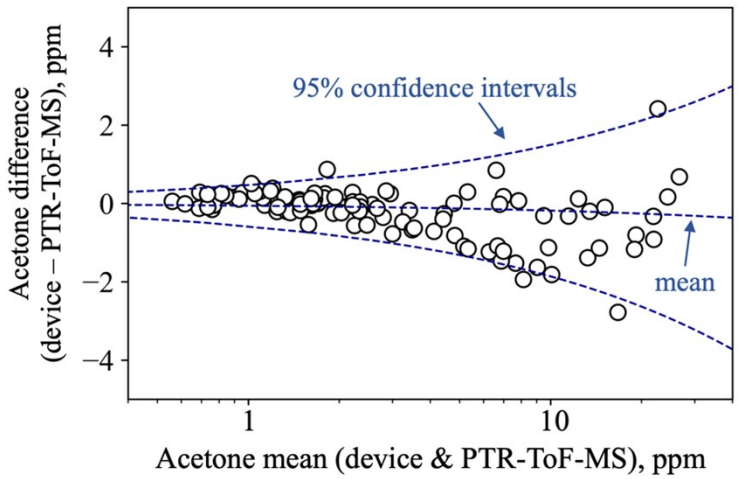

Figure S8: Bland−Altman plot showing the difference in acetone concentration measured using the device and the PTR-ToF-MS as a function of the mean of both measurements. The mean and the limit of agreement (95% confidence intervals) of these differences are indicated as dashed lines.

Table S1: Volunteer anthropometric data as well as estimated energy expenditures and target heart rates.

#	Age	Gender [m/f]	Weight [kg]	Height [cm]	REE* [kcal/d]	Calorie intake+ [kcal/d]	Target HR [bpm]
1	26	f	54	167	1294	1553	126
2	33	f	78	166	1493	1792	122
3	25	m	78	192	1856	2228	126
4	28	f	54	169	1297	1556	125
5	24	f	65	176	1470	1764	127

* Resting energy expenditure. + Calorie intake = REE × 75% × 1.6, where 1.6 was chosen for the physical activity factor.