Supporting Information

Dynamic breath limonene sensing at high selectivity

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Figure S1: Sensor response to 1000 ppb of hydrogen (red), methanol (green), carbon monoxide (CO, light green), ethanol (black), 2-propanol (brown), acetone (purple) and isoprene (turquoise), and 100 ppb limonene (blue) without (filled bar) and with (hatched bar) the separation column in air at 50% RH. Error bars correspond to three measurements recorded using separate separation column-sensor systems.



Figure S2: Retention time of the detector's limonene response as a single analyte (triangles) and in a gas mixture containing methanol, 2-propanol, hydrogen and acetone, each at 1000 ppb (circles) as a function of limonene concentration.



Figure S3: Sensor response to 20 - 500 ppb limonene in a gas mixture containing methanol, 2-propanol, hydrogen and acetone, each at 1000 ppb without (squares) and with (diamonds) the separation column as a function of limonene concentration. All measurements were performed in air at 50% RH.



Figure S4: Detector resistance upon three subsequent exposures to 100 ppb limonene in a gas mixture containing 4000 ppb interferants (methanol, 2-propanol, hydrogen and acetone, each at 1000 ppb).



Figure S5: Relative humidity (RH, squares, left ordinate) and temperature (circles, right ordinate), as measured in laboratory air during 20 days. The dashed lines indicate the average RH and temperature, while average values \pm STD are provided as well.



Figure S6: Detector response (triangles, left ordinate) and limonene retention times (circles, right ordinate) for 90, 180 and 270 s exposures to 100 ppb limonene in air at 50% RH.



Figure S7: Detector response (black, solid line, left ordinate) and corresponding limonene (blue, dashed, right ordinate), acetone (purple) and isoprene (orange) concentrations as measured with the PTR-ToF-MS at all timepoints for volunteer #1.



Figure S8: Scatter plot showing the detector response and limonene concentrations (by PTR-ToF-MS) for volunteer #1 (sample size N = 14).



Figure S9: Normalized detector response (black, solid line, left ordinate) and corresponding limonene (blue, dashed, right ordinate), acetone (purple) and isoprene (orange) concentrations as measured with the PTR-ToF-MS at all timepoints for volunteer #2. The detector normalization at t = 150 s (dotted horizontal line) is indicated for 15 min.



Figure S10: Normalized detector response (black, solid line, left ordinate) and corresponding limonene (blue, dashed, right ordinate), acetone (purple) and isoprene (orange) concentrations as measured with the PTR-ToF-MS at all timepoints for volunteer #3. The detector normalization at t = 150 s (dotted horizontalline) is indicated for 75 min.



Figure S11: Normalized detector response (black, solid line, left ordinate) and corresponding limonene (blue, dashed, right ordinate), acetone (purple) and isoprene (orange) concentrations as measured with the PTR-ToF-MS at all timepoints for volunteer #4. Note that during the first exhalation at t = 0 min, the volunteer did not maintain the exhalation for 30 s, but briefly stopped after 15 s before completing it. The detector normalization at t = 150 s (dotted horizontal line) is indicated for 15 min.