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Supplement of

Development of a gas chromatography system coupled to a metal-oxide semiconductor (MOS) sensor, with compensation of the temperature effects on the column for the measurement of ethene

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S1. Column characterization test measurements

Peak number 1 refers to air, which is introduced at the sample injection. Peak no. 2 refers to carbon dioxide (CO_2), peak no. 3 refers to ethene and sometimes there occurs a peak no. 4 (figure S1b, e and f), which refers to a baseline shift. This is due to humidity that is in the system and comes through the column after a certain while. Baking out the column eliminates the problem until new moisture reaches the detector during the course of the experiments. Besides a baseline shift, this has no further effect on the measurements.
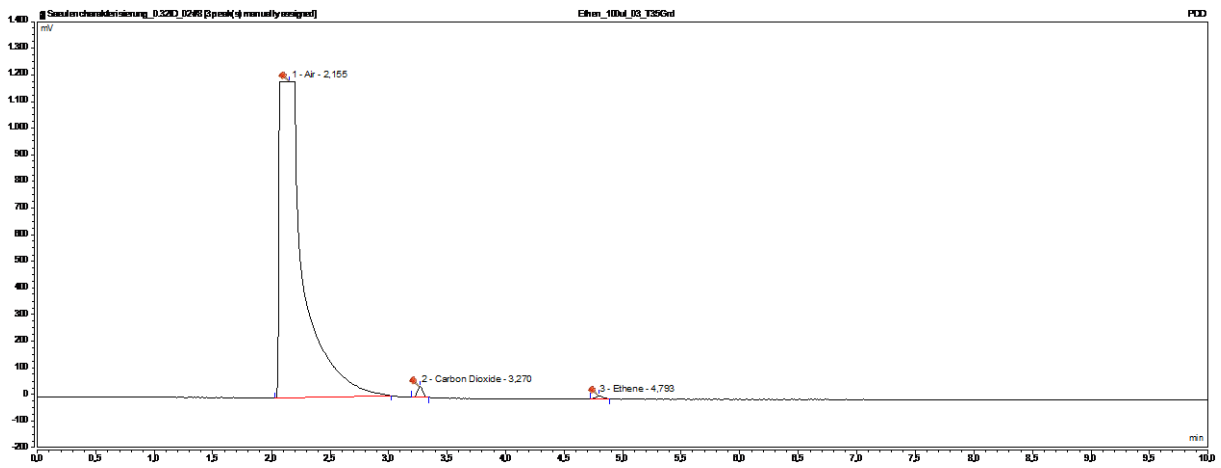
a) Blanc value:

b) 32 °C:

2

c) 35 °C:

3

d) 40 °C:

4

e) 45 °C:

5
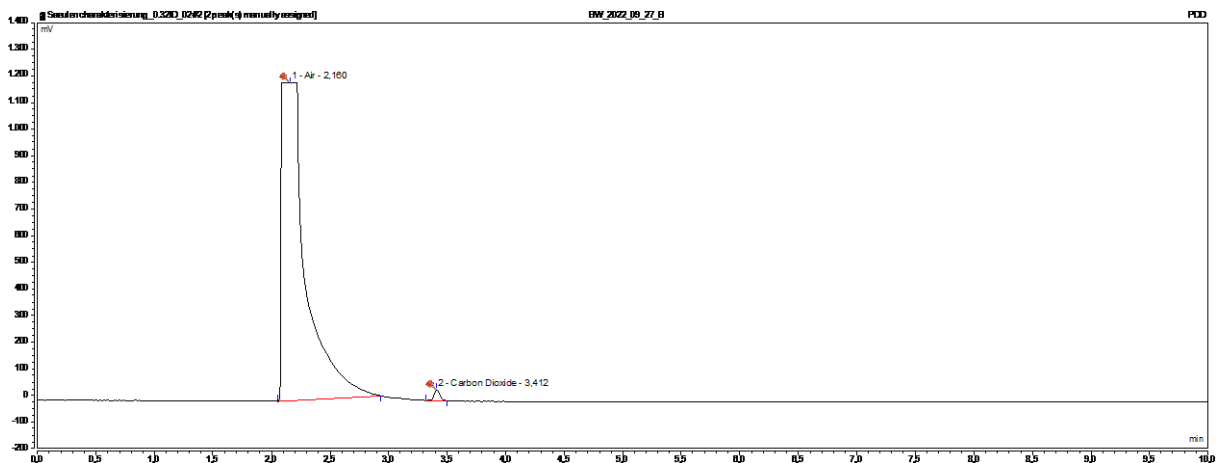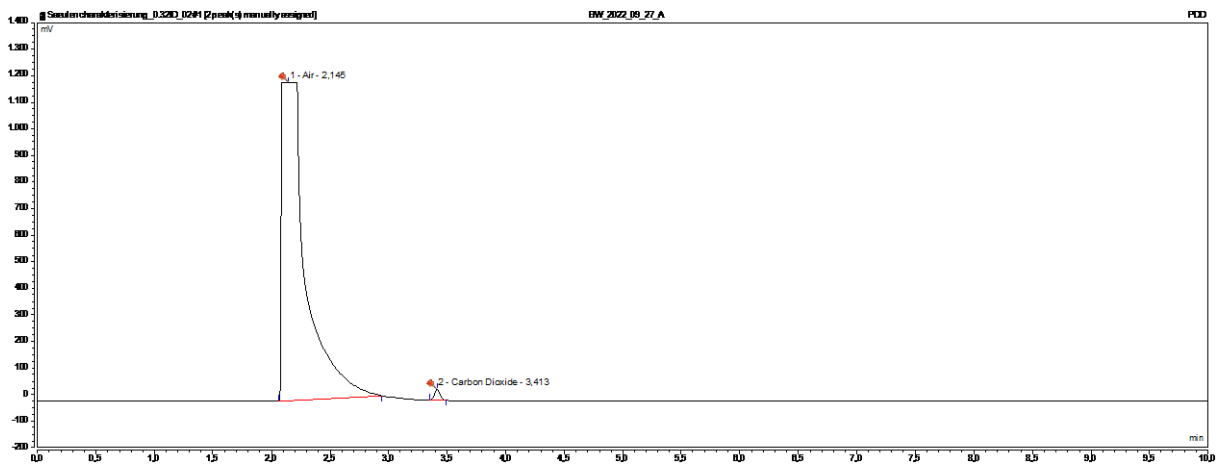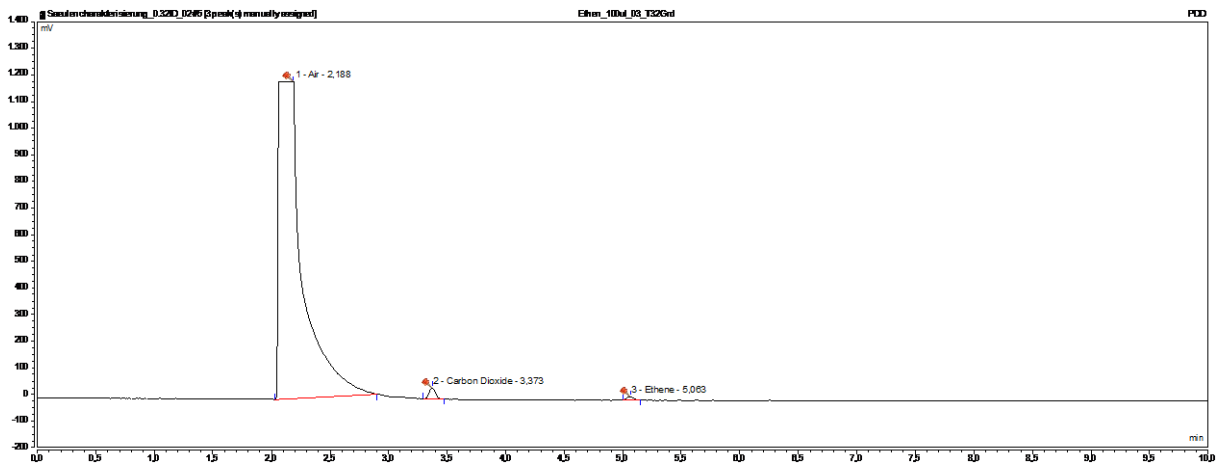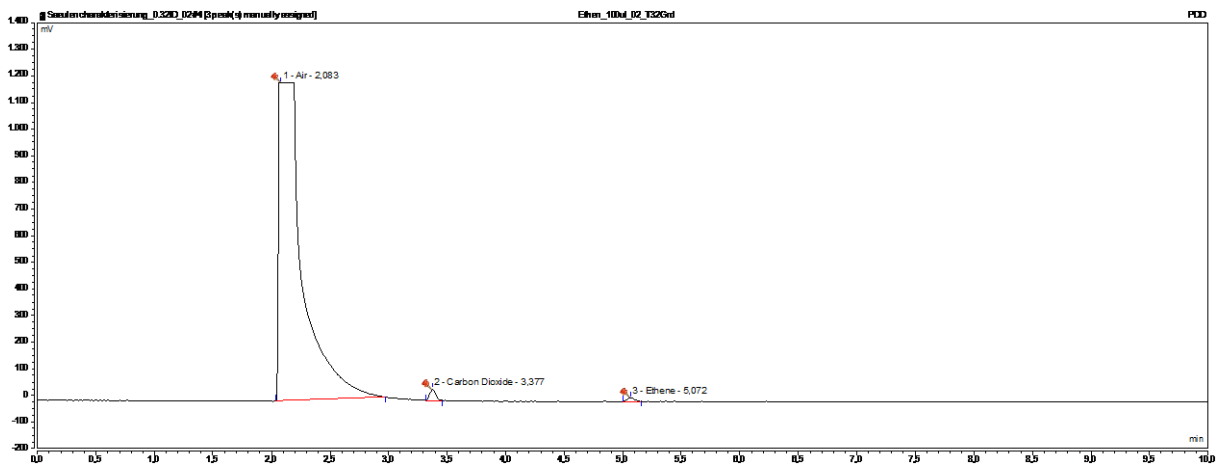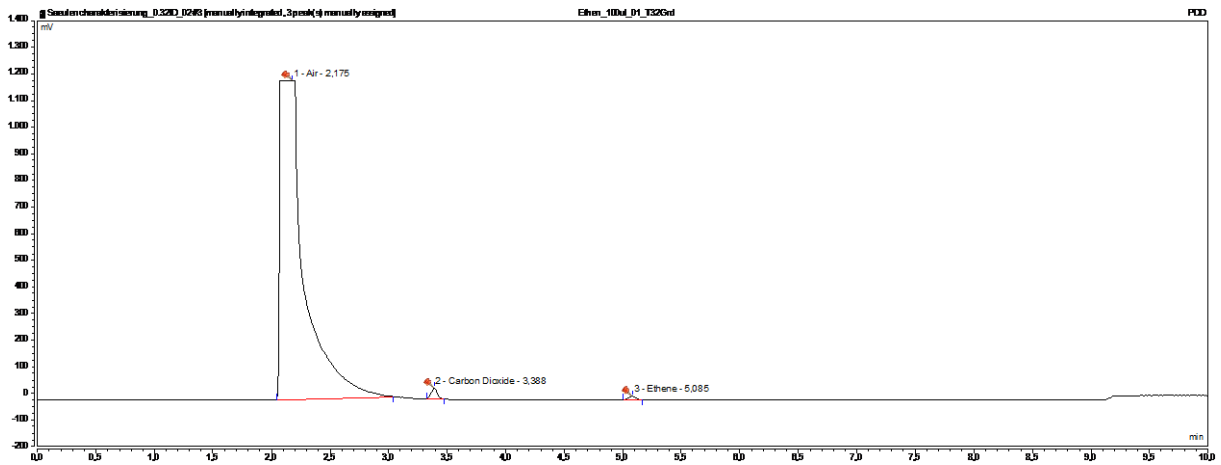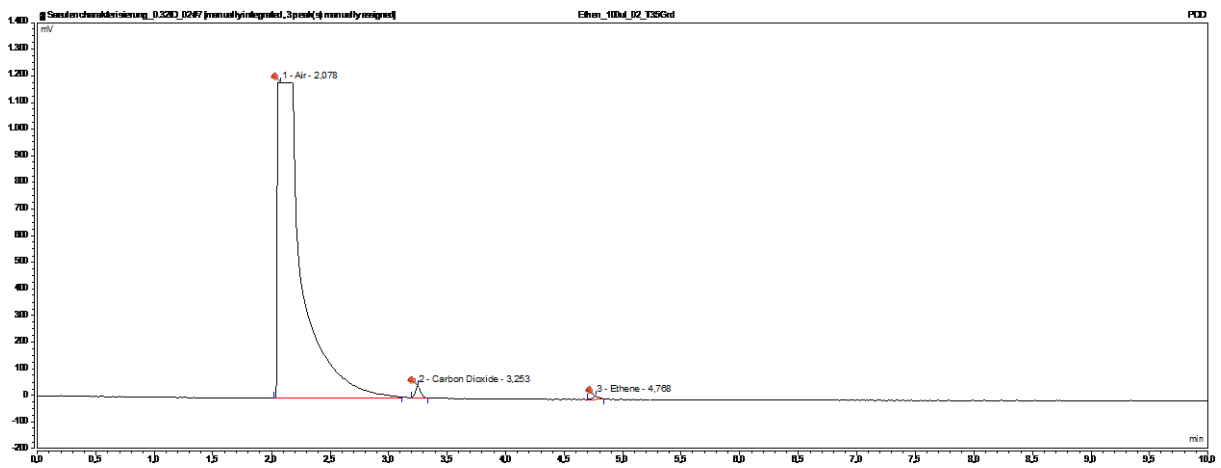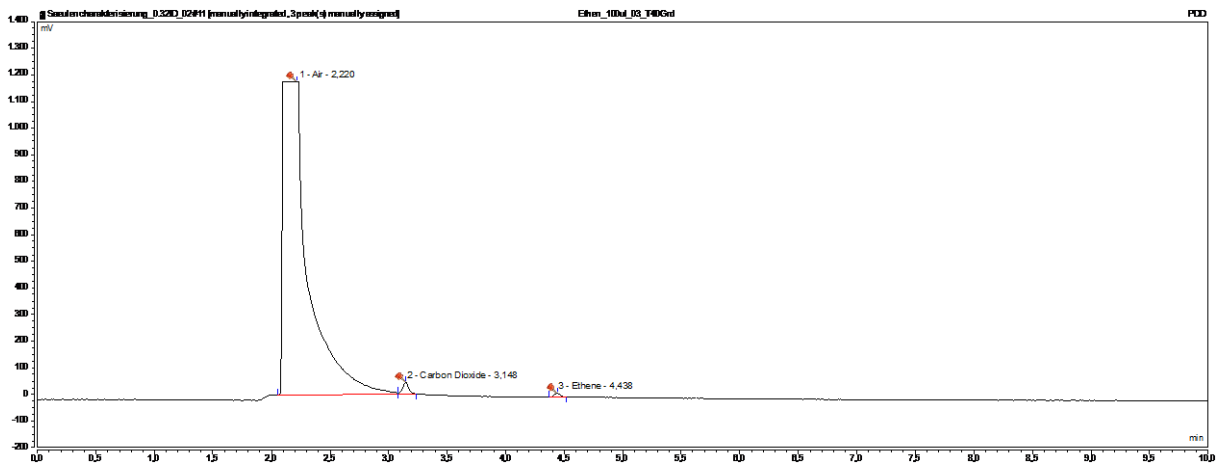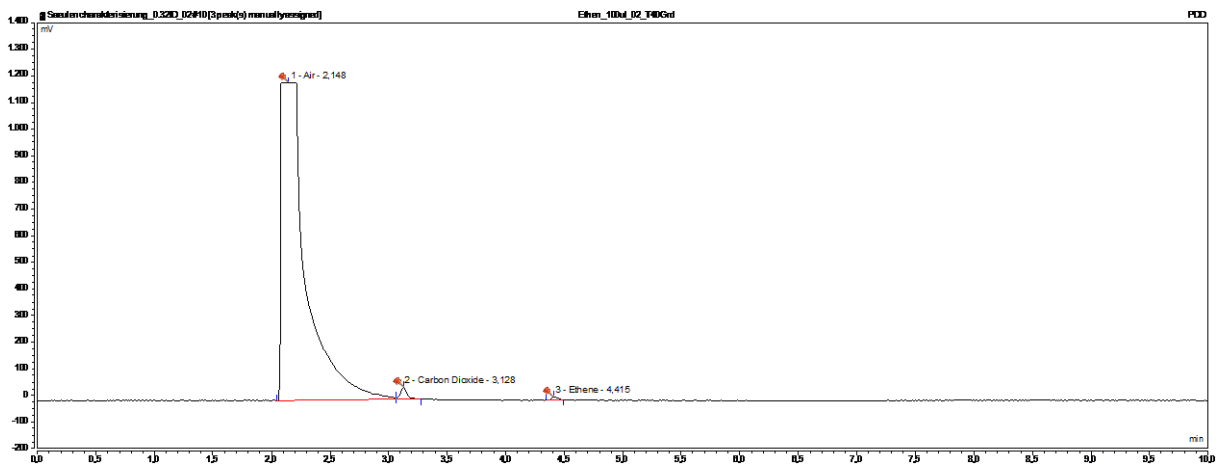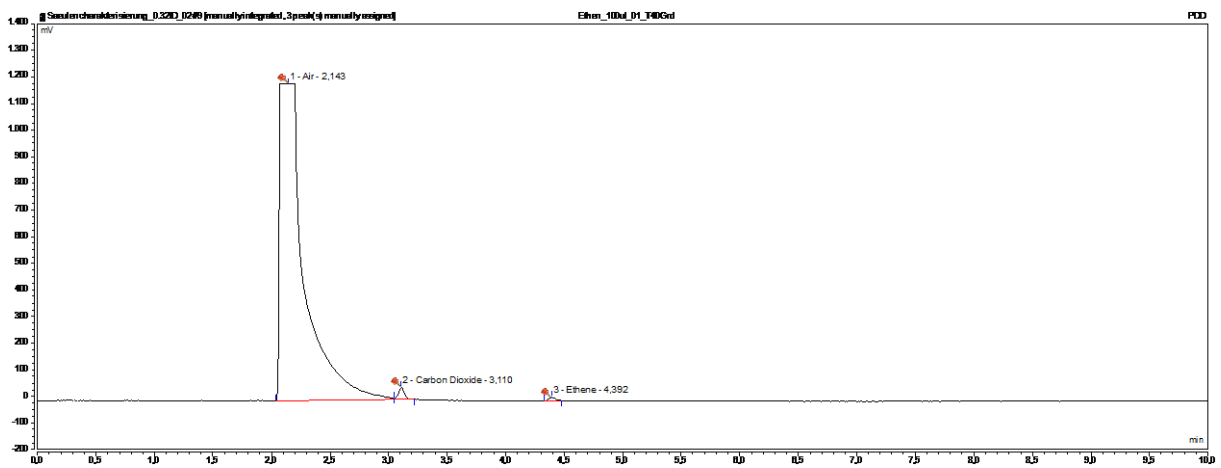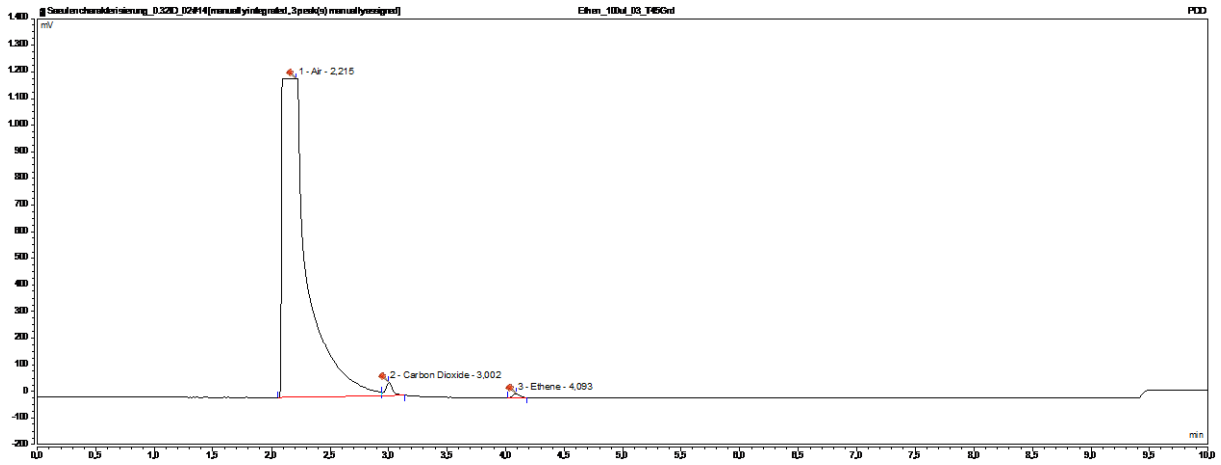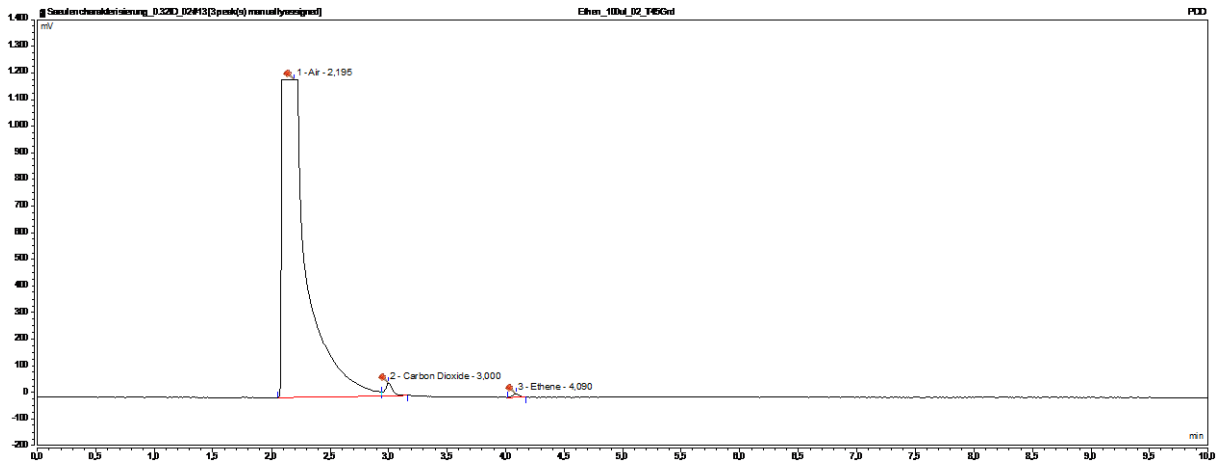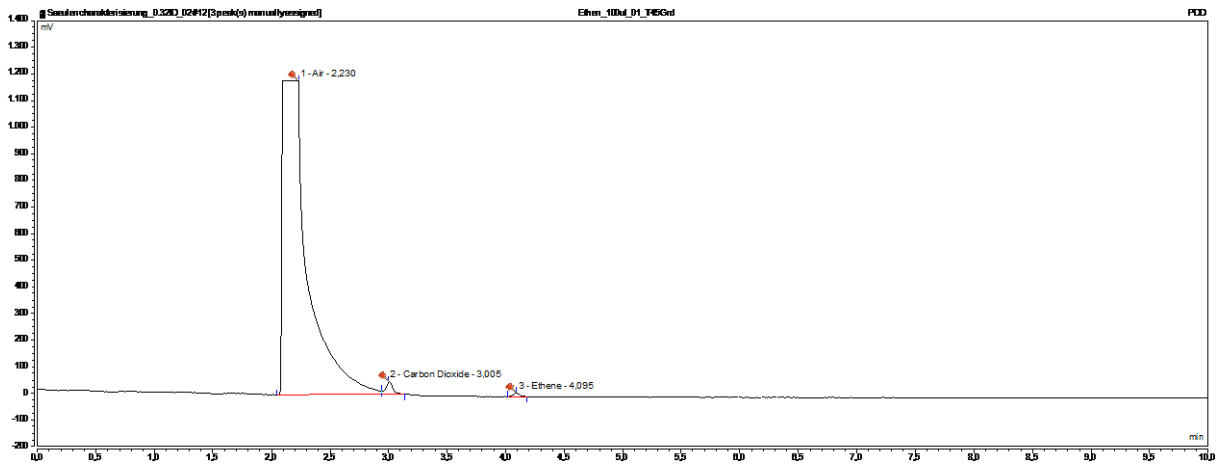
f) 50 °C:
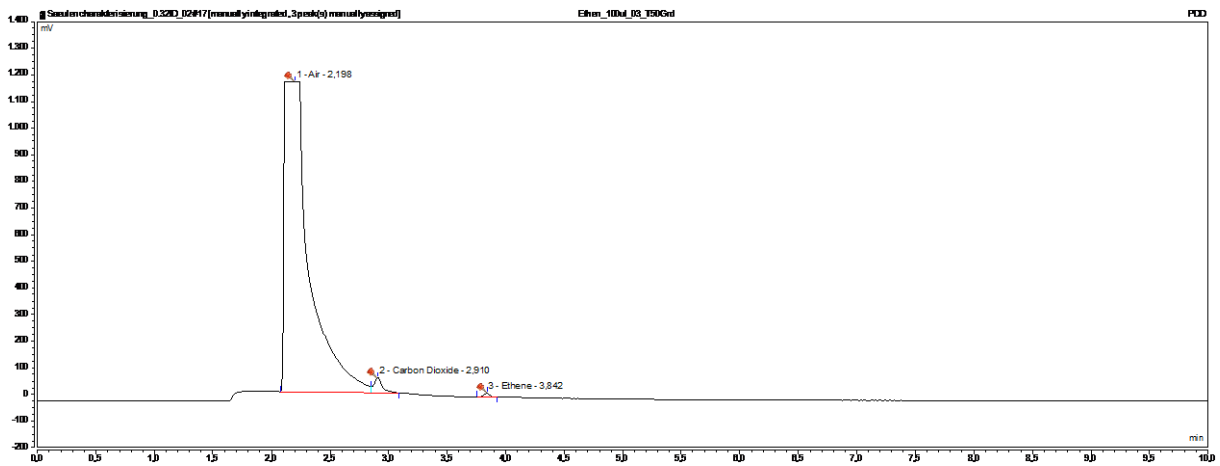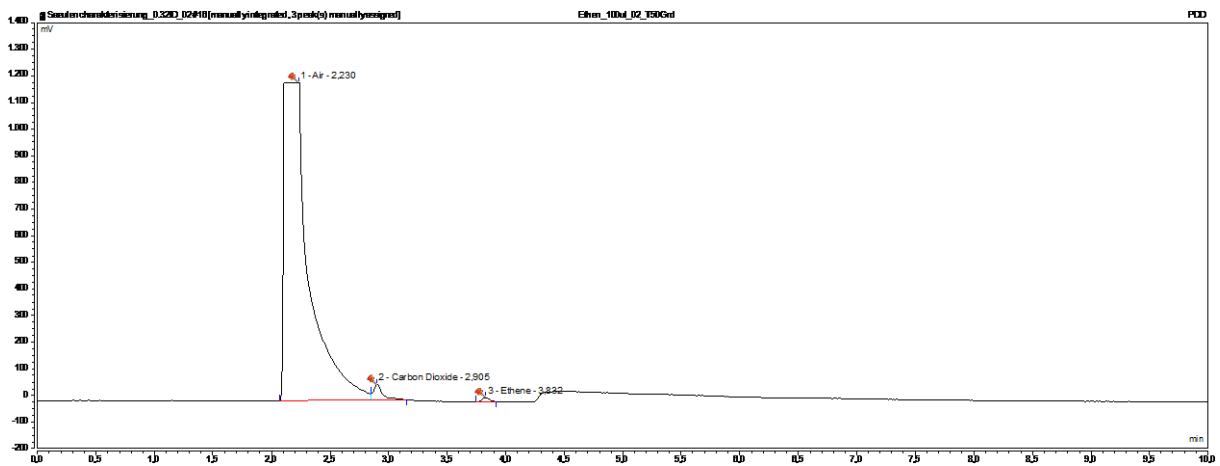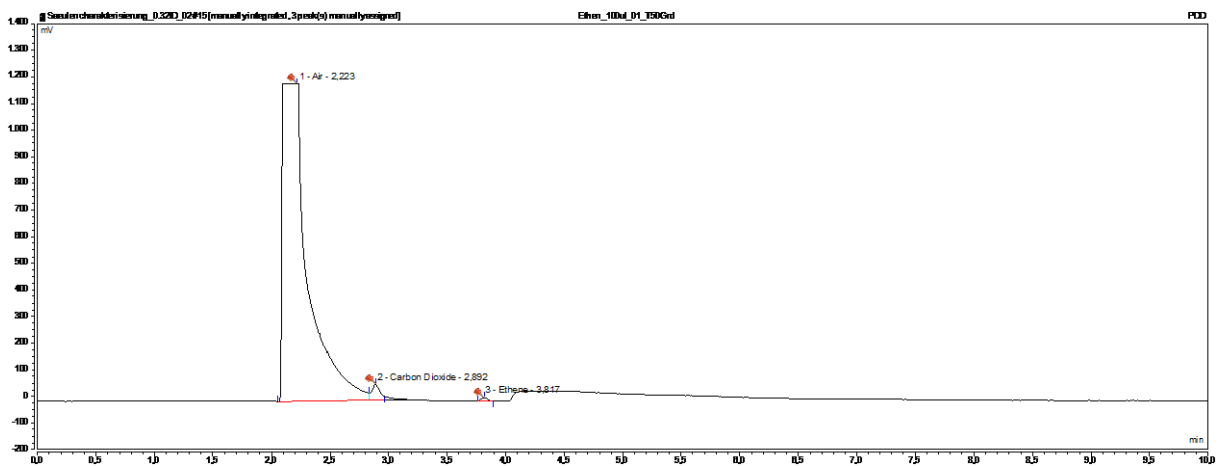
Figure S1: Chromatograms received from the column characterization measurement at a PDD-GC (pulsed discharge detector gas chromatography). a) blanc value (surrounding air); for b-f measurement with ethene/air mixture and b) 32 °C; c) 35 °C; d) 40 °C; e) 45 °C; and f) 50 °C.

Additionally, the values received from chromatograms were summarized in table S1:

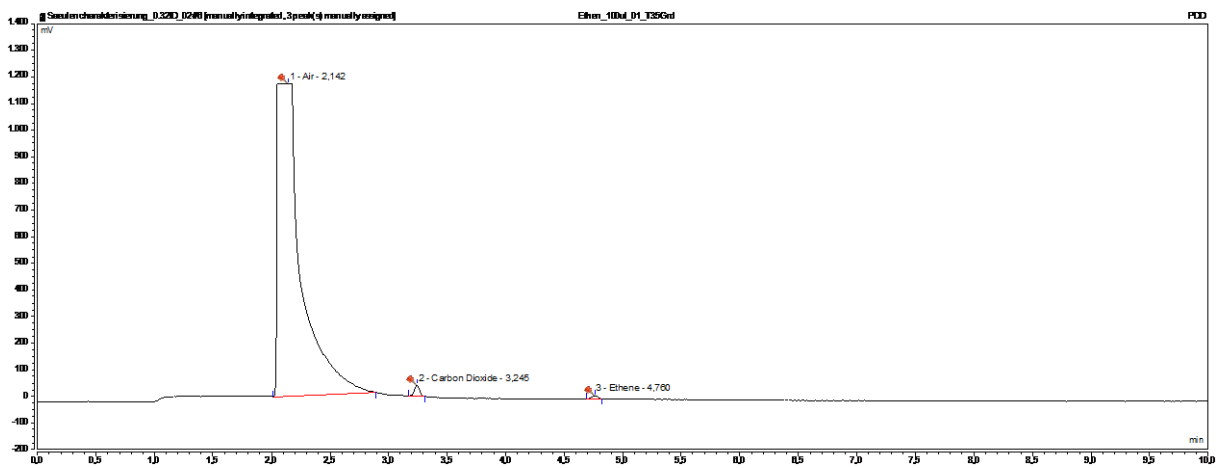Table S1: Measured retention times on a benchtop PDD-GC for column characterization.

| Temperature [°C]	Temperature [°K]	$t_r\ CO_2$ [min]	$t'_r\ CO_2$ [min]	$t_r\ Ethene$ [min]	$t'_r\ Ethene$ [min]
32	305.15	3.388	1.708	5.085	3.405
32	305.15	3.377	1.697	5.072	3.392
32	305.15	3.373	1.693	5.063	3.383
35	308.15	3.245	1.565	4.760	3.080
35	308.15	3.253	1.573	4.768	3.088
35	308.15	3.270	1.590	4.793	3.113
40	313.15	3.110	1.430	4.392	2.712
40	313.15	3.128	1.448	4.415	2.735
40	313.15	3.148	1.468	4.438	2.758
45	318.15	3.005	1.325	4.095	2.415
45	318.15	3.000	1.320	4.090	2.410
45	318.15	3.002	1.322	4.093	2.413
50	323.15	2.892	1.212	3.817	2.137
50	323.15	2.905	1.225	3.832	2.152
50	323.15	2.910	1.230	3.842	2.162

S2. Graphical user interface:

Based on the temperature compensation algorithm (TCA) a graphical user interface (GUI) is currently in development to achieve a user-friendly practicability. Therefore, Eq. (6) was transformed into a MATLAB based script. Underlying parameters, such as gas flow, column diameter or column length, can be variably adapted to the column used. The retention values from the characterization measurement of the corresponding column can be entered into an underlying Excel-table. The sorption parameters S and H are then automatically calculated for the corresponding gases and a prediction of the retention time of the test gas depending on the reference gas is possible (green field). Additionally, test and reference gases are selectable, so that the usage of the GUI can be extended for future applications and different gases. At the current status, the GUI is only able to predict the benchtop GC values, as just the carrier gas stream and one detector needs to be considered there. However, further adjustments of the GUI will be made to the respective GC set-up and target applications.
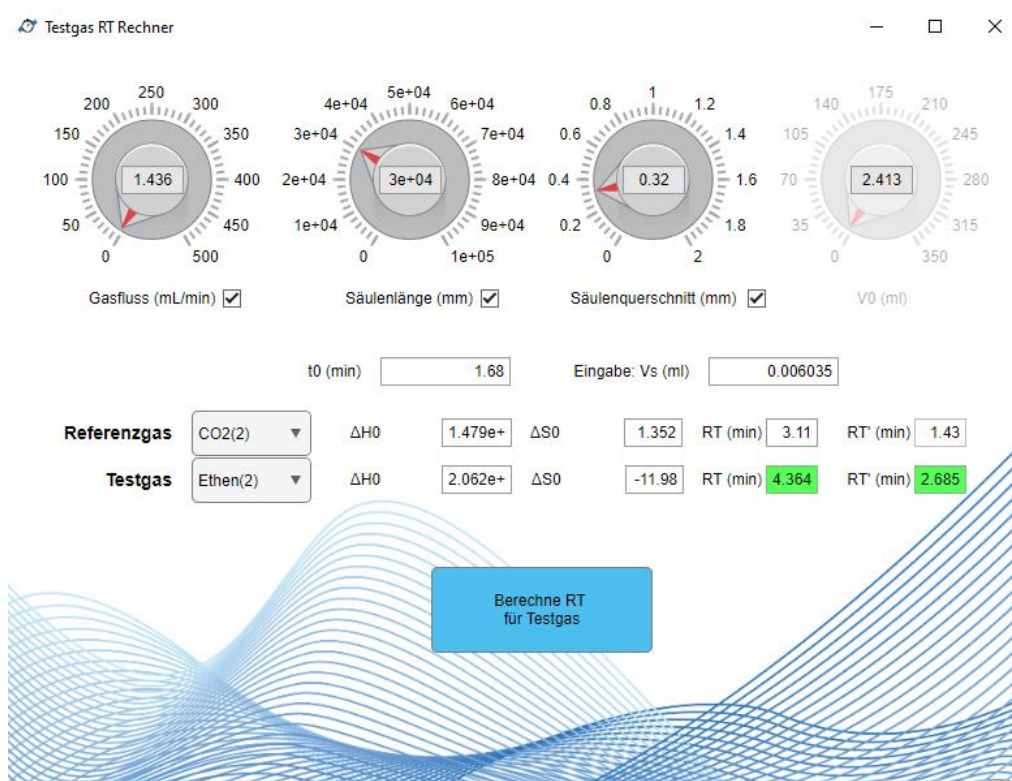

Figure S2: Screenshot of the graphical user interface, version 2023_02_14. Adjustable parameters are gas flow (Gasfluss), column length (Säulenlänge), and column diameter (Säulenquerschnitt). Predicted values are highlighted in green (RT' = net retention time; RT = gross retention time).

S3. Peak detection:

The peak detection was performed using the library '*peakdetect*' (https://github.com/avhn/peakdetect). It checks not only the absolute maxima or minima of a signal, but also if there are any L points before and after the detected peak, with L being the parameter for deciding how many points to be considered. This should ensure that the selected peak maxima is a point lying between valleys and the minima is a point lying in a valley surrounded by other signal points for both cases. Thus the algorithm checks that each candidate peak within the given signal is an actual peak by comparing if there are any peaks within this given window of 2 L points. Additionally, the algorithm also requires a Delta (D) parameter that can be used to check if the peak found is noise or in fact an actual peak. Parameter D is the minimum difference between a peak and the points within this window of length 2 L. For the given data, the parameters L and D were found experimentally.

For the CO_2 peaks parameter D was varied from 0 to the RMS (Root Mean Square) of each of the signals and the false peaks detected were counted. Similarly, L was varied from 1 to half the length of the signal. The combinations of L and D that lead to the least false positives were chosen as the optimal parameters for our use-case. L was set as 2 and D was set as 8. Similarly, the troughs were identified for the Ethylene sample using a similar strategy. Here, parameter D was experimentally found by varying it from 0 to twice the RMS value of the signals. D was then set as 1.5 * RMS value and L window size was set as 10, as this lead to detection of all the peaks in the data and no false detections. peaks were calculated as shown in the following example for CO_2 (figure S3a) and ethene (figure S3b and S3c).

a)

```
all_peaks_with_large_lookahead = []
for file in co2_files:

all_peaks_with_large_lookahead.append(find_peak_and_times(os.path.join(path_to_data
,file), plot=True, lookahead=2, delta='RMSE', debug=True))

Max Peak at: Rel Time: 00:04:38.5079814s intensity: 891
Lookahead: 2, siglen: 1364, delta: 424.9378969633796
RMSE: 424.9378969633796, Mean: 413.5065982404692, Max: 891, Min: 376
No lower peaks found
```
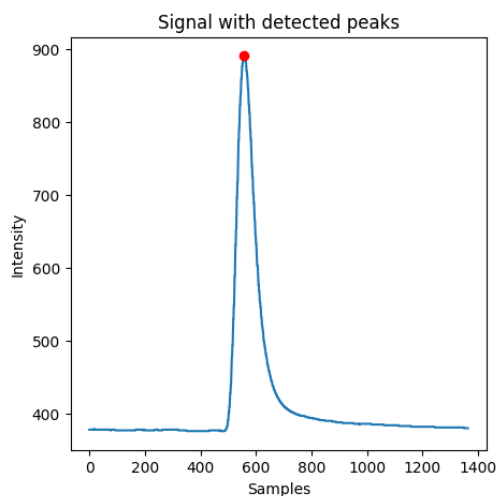

b)

```
for files in h5_files:
    print(f"For file: {files}")
    sen, ts = create_sensor_vector(os.path.join(file_dir, files))
    find_peak_and_times_data(sen, timesteps=ts, lookahead=10, delta='1.5*rmse',
debug=True, save_index=files)

For file: 2022_08_08_HM01_150ul_MU.h5
Peak 1: Rel Time: 1659973333413046s intensity: 50996, Index: 2363
Lookahead: 10, siglen: 5999, delta: 272.39336855524243
RMS: 181.5955790368283, Mean: 54888.53325554259, Max: 55391, Min: 50996
```
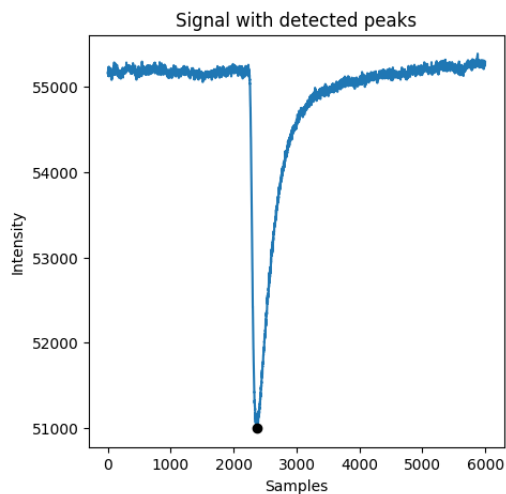

c)

```
For file: 2022_08_10_SGM01_150ul_MU.h5
Peak 1: Rel Time: 1660145062613046s intensity: 54470, Index: 1565
Peak 2: Rel Time: 1660145146213046s intensity: 53109, Index: 2401
Peak 3: Rel Time: 1660145173713046s intensity: 53492, Index: 2676
Lookahead: 10, siglen: 5999, delta: 272.0166188369513
RMS: 181.34441255796753, Mean: 55088.35205867644, Max: 55494, Min: 53109
```
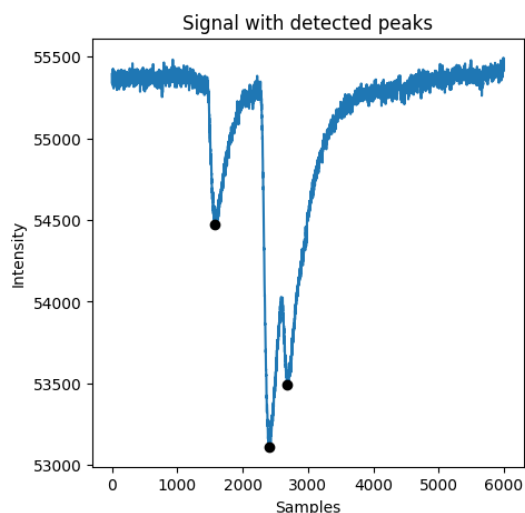

Figure S3: Peak detection shown for: a) CO_2 (ethene/air mixture); b) ethene (ethene/air mixture); and c) volatile compounds (ethene/interfering gas-mixture).

S4. Real sample measurements

Real sample measurements based on previously work (Köhne et al. 2021) were performed using the benchtop PDD-GC (Fisons Instruments, GC 8000 series). A PLOT column (GS-Q Megabore, 0.53 mm ID, Agilent, USA) at 32 °C and a PDD (VICI -Valco Instruments Co. Inc., USA) were used, while Helium served as carrier gas stream. The measurements are based on Köhne et al., 2021 and were performed with avocados (weighed portion of 837 g) and apples (weighed portion 322 g), which were stored in a gastight glass cylinder (4 L Volume) for nine days and three days respectively. The apple measurement revealed a stronger ethene emission than the avocado measurement (figure S4a). Therefore, a measurement of apples with different column temperatures were performed in addition, starting at 32 °C (lover limit of GC oven), 35 °C, 40 °C, 45 °C, 50 °C, 60 °C and 70 °C (figure S4b). Both fruits showed an enormous CO_2 level in the first experiment (at PDD detector limit), due to cellular respiration of fruits. No further gases could be observed in both experiments. With rising temperature, CO_2 peaks and ethene peaks are moving closer to the air peaks. Moisture can be seen for 50 °C and for 60 °C as baseline shift, which is due to stored fruits.
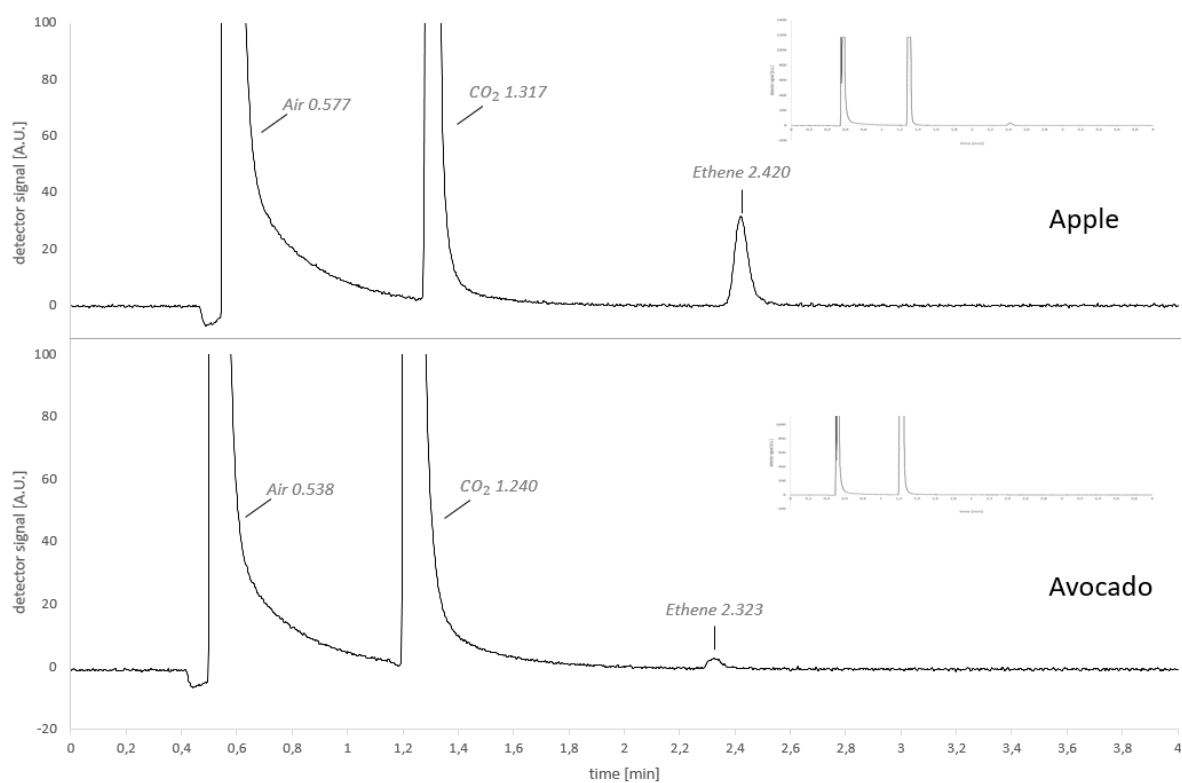

Figure S4a: Fruit measurement at 32 °C column temperature of apples stored for three days (upper graph) and avocados stored for nine days (lower graph).
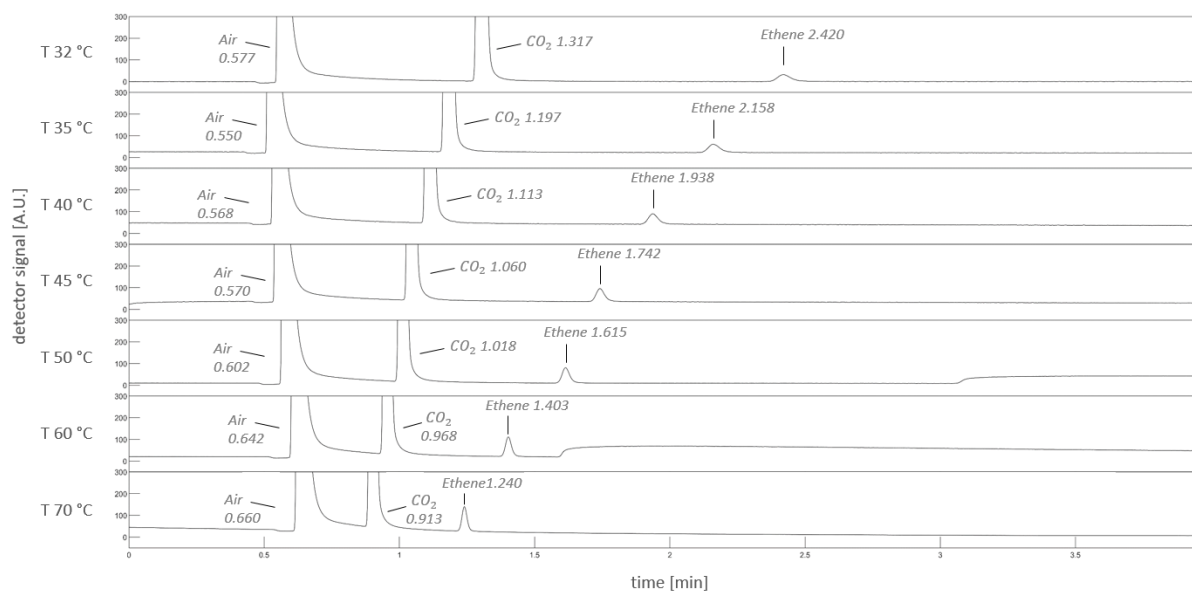
Figure S4b: Fruit measurements of apples stored for three days, at different temperature, downwards 32 °C, 35 °C, 40 °C, 45 °C, 50 °C, 60 °C and 70 °C. For 50 °C and 60 °C a baseline shift occurs, which is due to moisture originating from stored fruits.