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Supplement of

A versatile development platform for odor monitoring systems

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S1. Mass trace peak assignment

When comparing the chromatogram with a blank measurement, the pentane peak occurs to lay on the second air peak. Nevertheless, it can be clearly assigned to pentane and distinguished from the air peak based on the chromatogram of the mass trace 72 (for pentane), which does not show a peak in the blank measurement (Figure S1). As fragments of hexanal and octanal also have the same mass, those peaks are slightly visible as well in here.

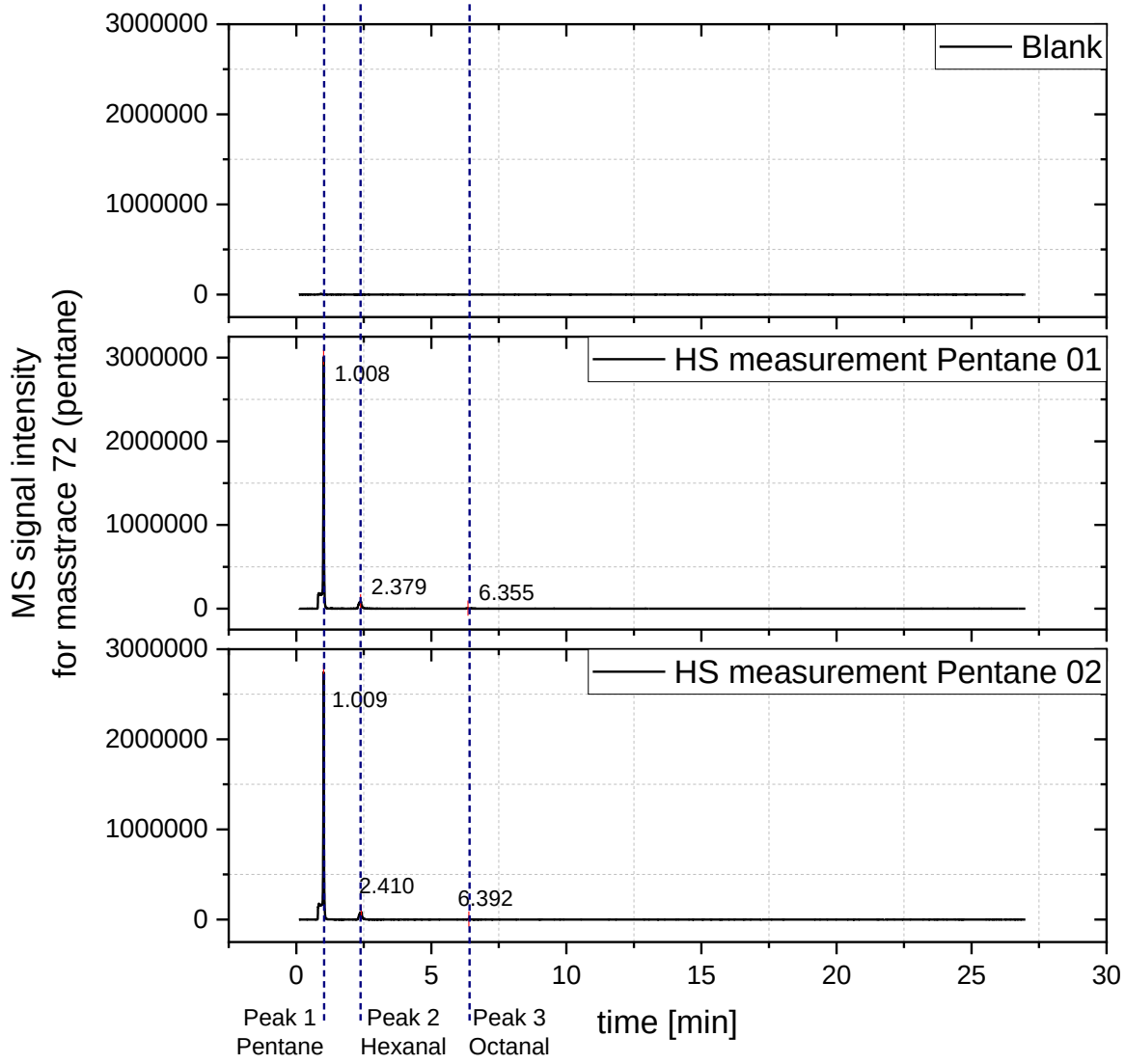

Figure S1: Comparison of mass traces in the mass spectrum (MS) signal for pentane (72). Top: a blank measurement (surrounding air); middle: headspace (HS) measurement of pentane (4 µL); bottom: replicate of the headspace measurement of pentane (4 µL).

S2. Semi-quantitative analysis of the peak areas

In previous reported measurements, layer 1 showed a less intense pentane peak, compared to the hexanal peak (Koehne et al. 2024). In the measurements carried out for this work, the pentane peak was slightly more intense than the hexanal peak, although both measurements used the same samples and the same method. In order to identify a possible contamination with pentane, the peak areas of both measurements were compared to each other (Table S1 and Figure S2). Thereby, the pentane peak offers a clear increase in the peak area, indicating a possible contamination.

Table S1: Peak area comparison of previous measurements (Koehne et al. 2024) and measurements conducted for this work. Peak areas are given as mean value for all measurements.

	Peak areas from previous measurements (Koehne et al. 2024) [counts*min]	Peak areas from measurements conducted for this work [counts*min]
Peak 1 (Argon)	506,245	1,191,412
Peak 2 (Pentane)	1,029,571	3,015,377
Peak 3 (Hexanal)	212,177	274,025
Peak 4 (Octanal)	86,510	56,663

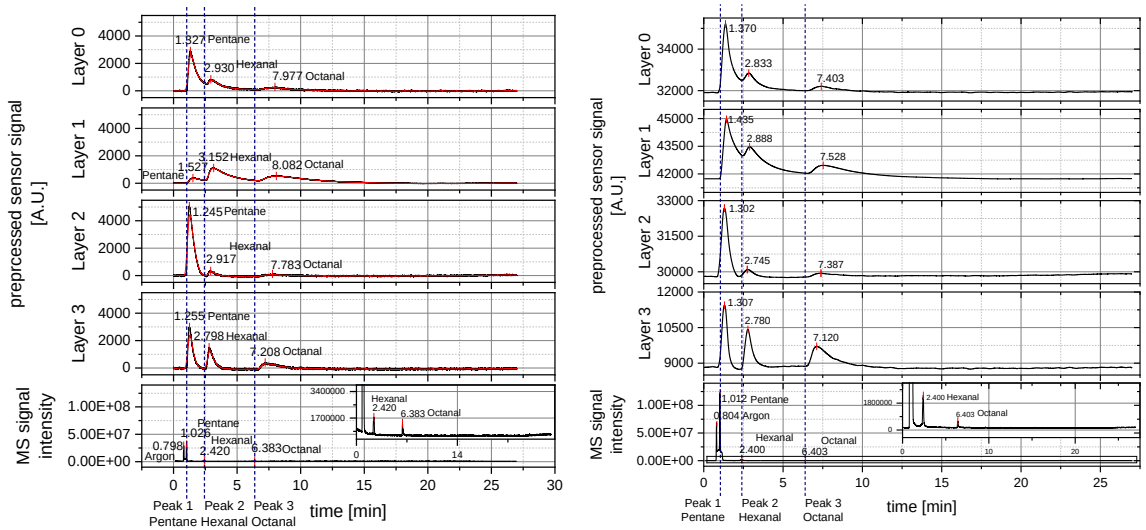

Figure S2: Comparison of the previous measurements reported at (Koehne et al. 2024) and the measurements reported here; left side: previous measurements translated and modified for the same visualization, black curve raw signal and red curve preprocessed raw signal; right side: measurements reported here. Both measurements used the same sample for injection to the GC and both sensor operation temperatures were set to 400 °C. MS = mass spectrometer.

S3. Chromatograms for each measured temperature step (100 °C – 400 °C)

The sensor was operated at different temperatures, to improve the sensor signal. Therefore, the sensor was operated starting with 100 °C and raising in 50 °C steps to 400 °C, starting 1 h with the respective temperature before each measurement was recorded. In addition, the sensor was operated at 100 °C for 15 h, before the measurement was recorded, afterwards the sensor was operated at 400 °C for 1 h, before the measurement at 100 °C was started (DSR-mode). An overview of all measurements can be found in Figure S3-S11. The MS chromatogram has been enlarged for an easier and clearer presentation. The full MS chromatogram is also shown in Figure S10.

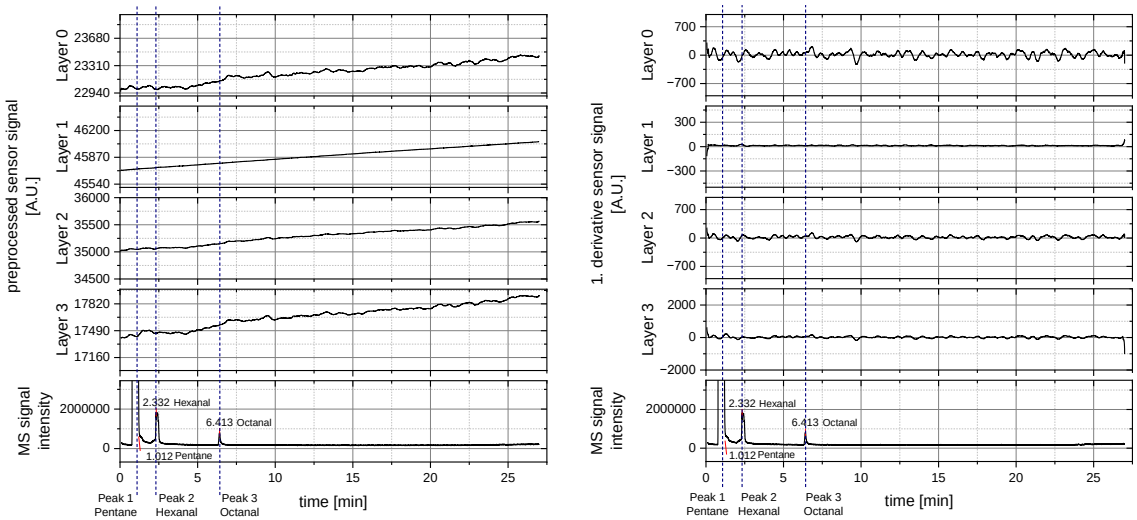

Figure S3: Measurement at 100 °C sensor temperature; left side: preprocessed raw signal, right side: first derivative of the preprocessed raw signal. MS = mass spectrometer.

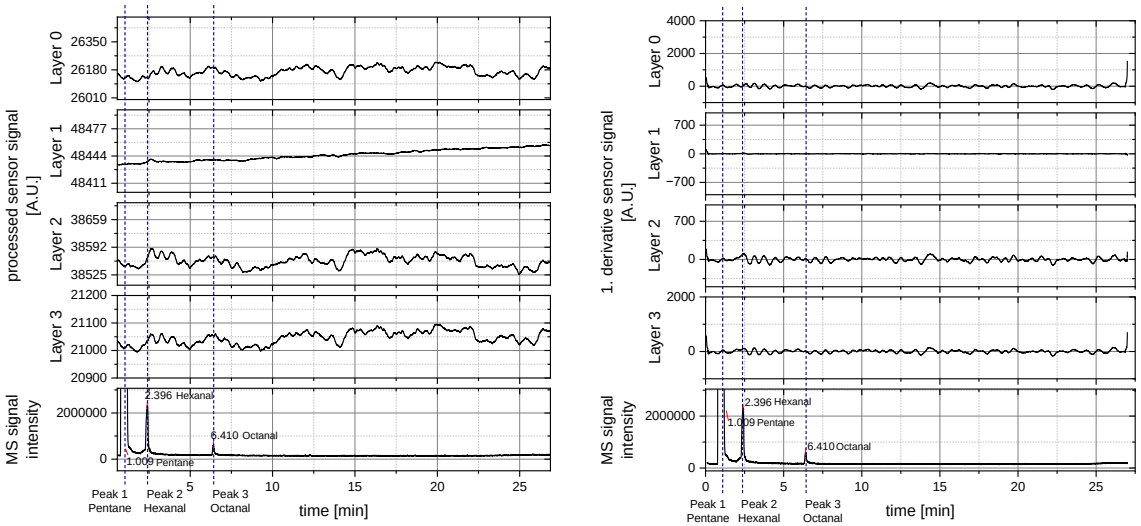

Figure S4: Measurement at 100 °C sensor temperature with a pre-operation at 100°C for 15h; left side: preprocessed raw signal, right side: first derivative of the preprocessed raw signal. MS = mass spectrometer.

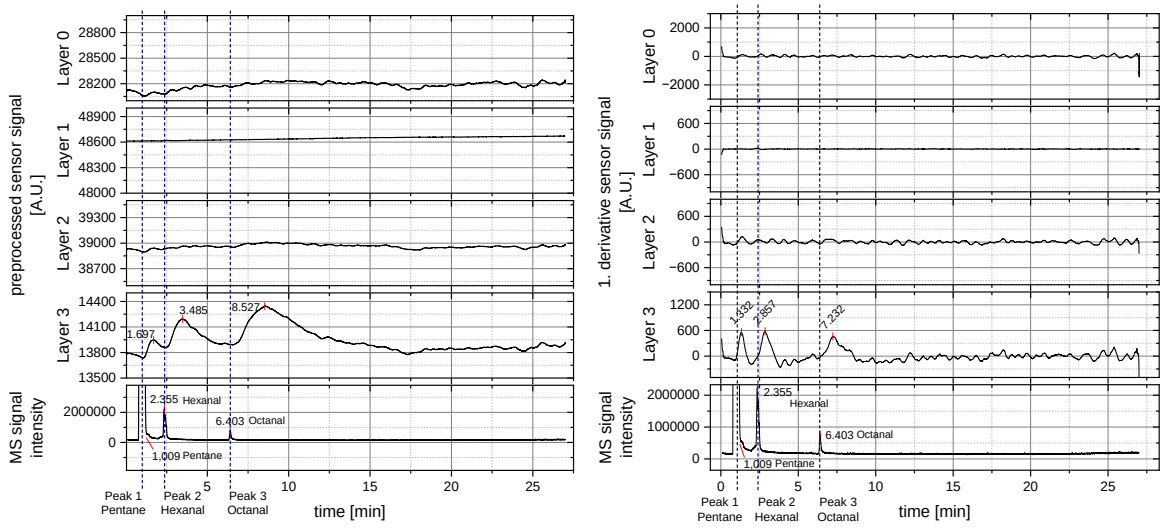

Figure S5: Measurement at 150 °C sensor temperature; left side: preprocessed raw signal, right side: first derivative of the preprocessed raw signal. MS = mass spectrometer.

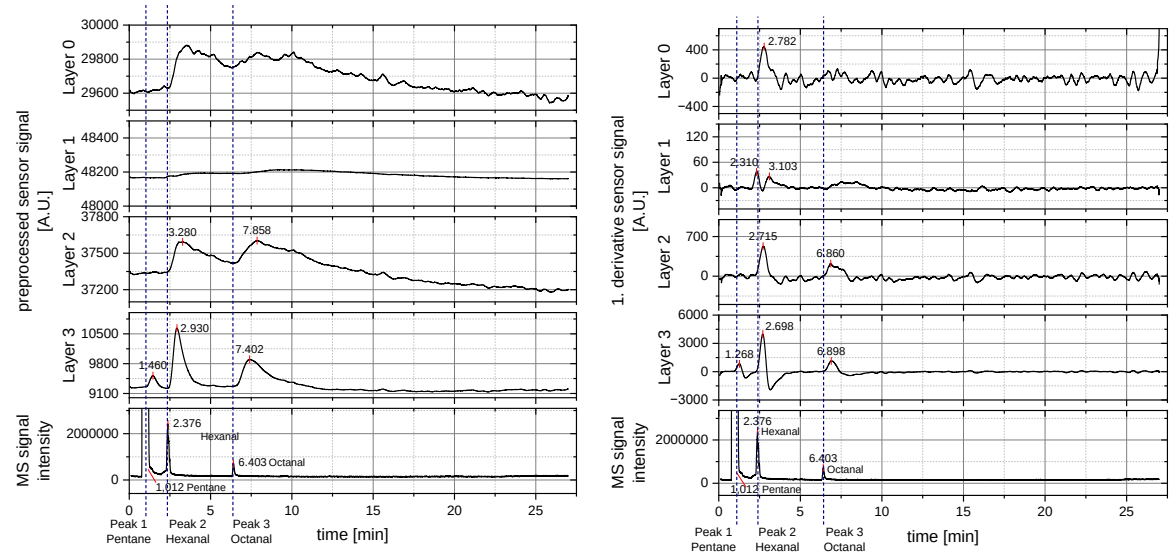

Figure S6: Measurement at 200 °C sensor temperature; left side: preprocessed raw signal, right side: first derivative of the preprocessed raw signal. MS = mass spectrometer.

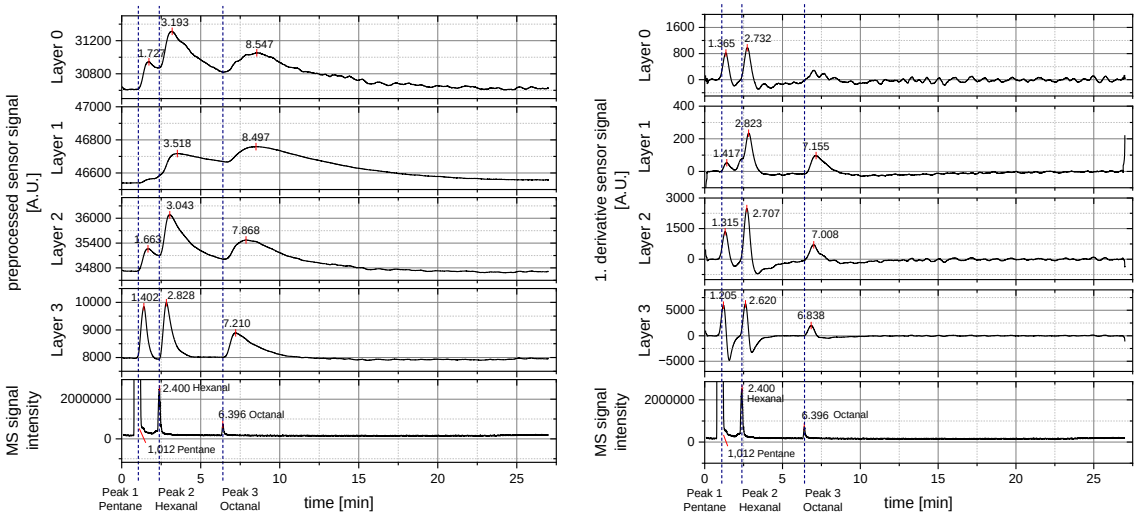

Figure S7: Measurement at 250 °C sensor temperature; left side: preprocessed raw signal, right side: first derivative of the preprocessed raw signal. MS = mass spectrometer.

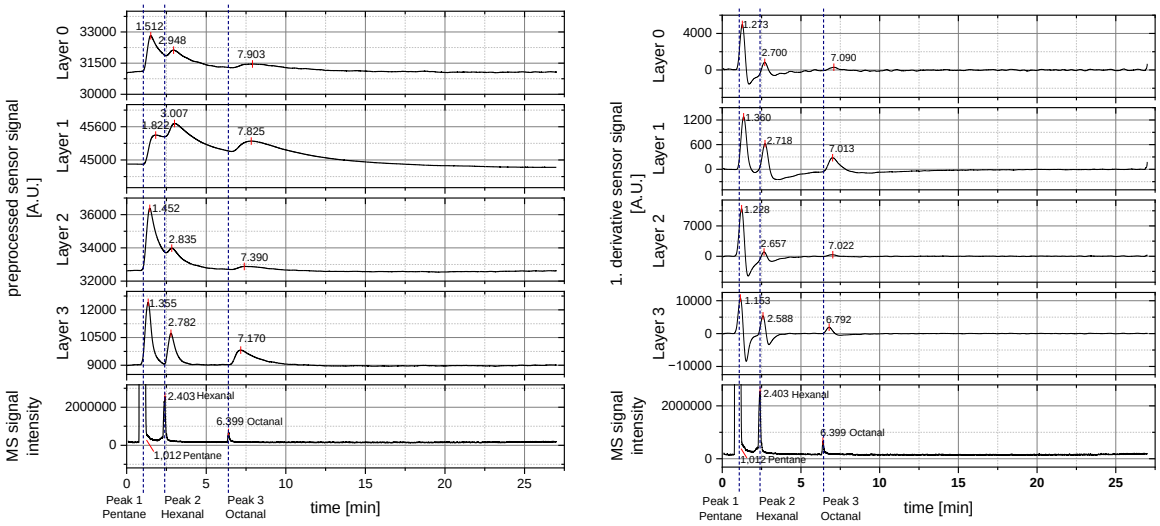

Figure S8: Measurement at 300 °C sensor temperature; left side: preprocessed raw signal, right side: first derivative of the preprocessed raw signal. MS = mass spectrometer.

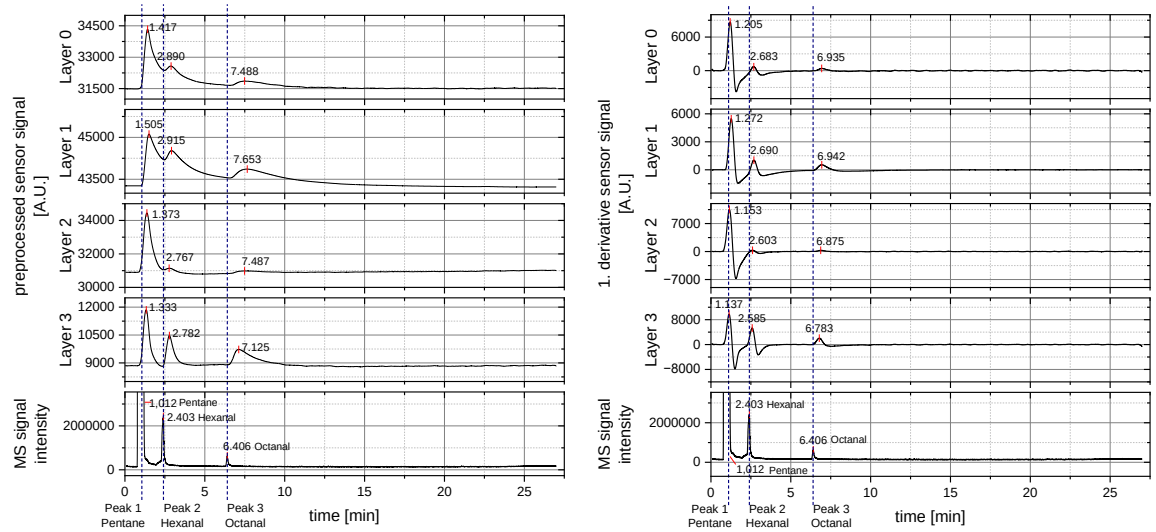

Figure S9: Measurement at 350 °C sensor temperature; left side: preprocessed raw signal, right side: first derivative of the preprocessed raw signal. MS = mass spectrometer.

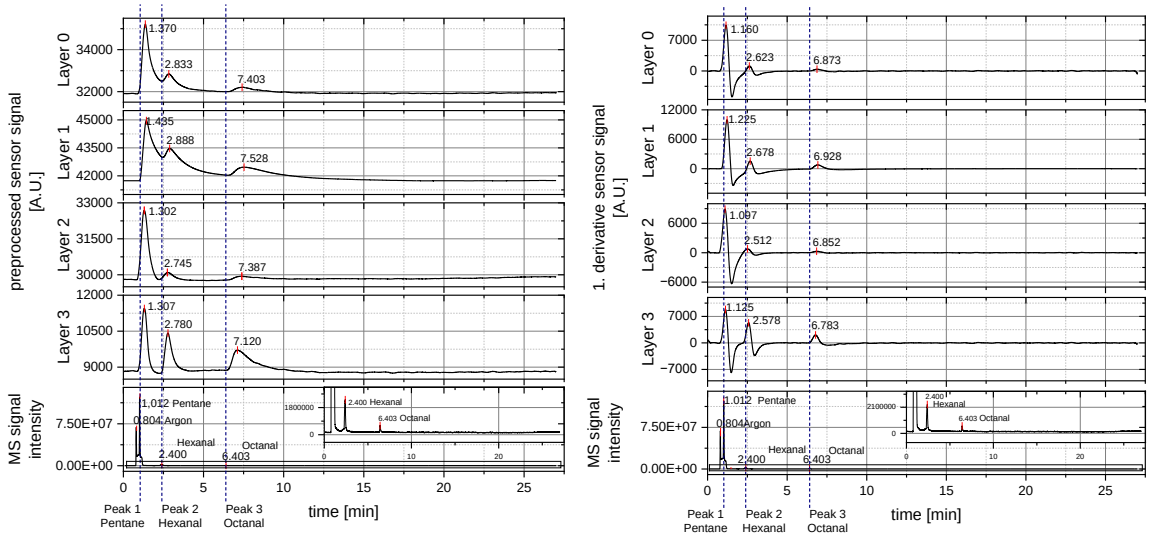

Figure S10: Measurement at 400 °C sensor temperature; left side: preprocessed raw signal, right side: first derivative of the preprocessed raw signal. MS = mass spectrometer.

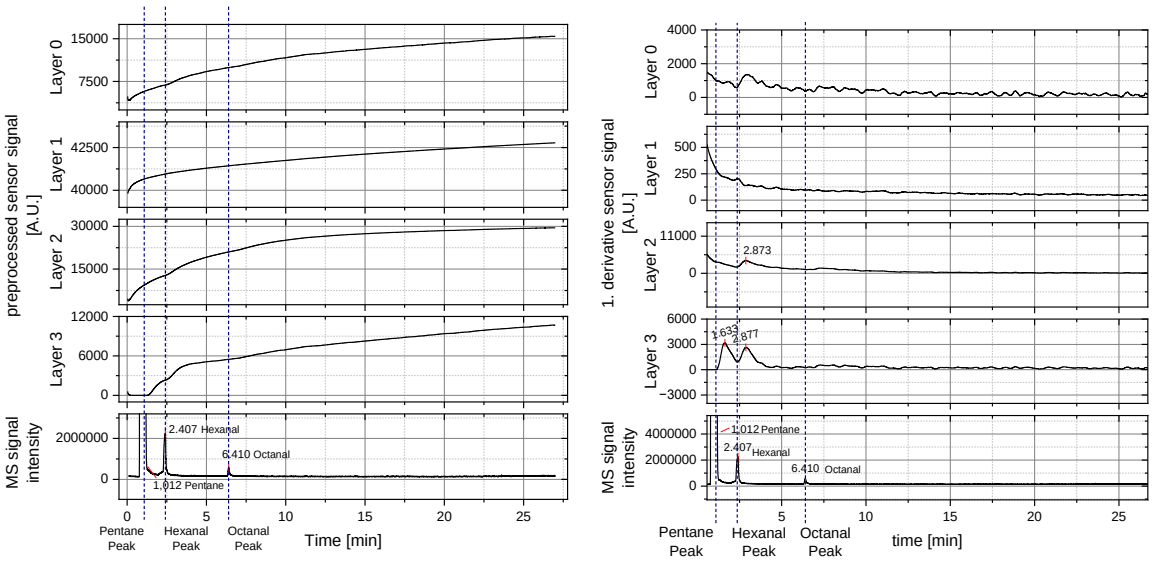

Figure S11: Measurement at 100 °C with the DSR-mode; left side: preprocessed raw signal, right side: first derivative of the preprocessed raw signal. MS = mass spectrometer.