Electronic Supplementary Material (ESI) for Analytical Methods.
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Electronic Supplementary Information

Discrimination of Structurally Similar Odorous Molecules with Various Concentrations by a Nanomechanical Sensor

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Supplementary Notes

Calculation of van der Waals (vdW) volume.

A van der Waals volume of each chemical is calculated by modified equation based on Bondi radii[1,2] as following equation (S1):

$$\text{vdW Volume (Å)} = \sum(all\ atom\ comtributions) - 5.92N_B - 14.7R_A - 3.8R_{NR} \qquad \text{(S1)}$$

where N_B, R_A and R_{NR} indicate the number of bonds, the number of aromatic rings and number of non-aromatic rings. N_B can be simply calculated by $N_B = N - 1 + R_A + R_{NR}$, where N is the total number of atom. Calculated vdW volumes of different series of molecules are shown in Fig. S1.

Calculation of saturated vapor pressure

A saturated vapor pressure [mmHg] of each chemical was estimated by Antoine equation (S2) as follow:

$$\log P_o = A - \frac{B}{t + C} \qquad \text{(S2)}$$

where t is temperature [°C], and A, B and C are constant of each chemical reported in Ref. 3. The constants of *A, B and C* are shown in Table. S1 in this ESI†. This equation can be used in the specific temperature range, which is also listed in Table. S1. In this study, we produced each vapor at 15 °C with bubbling. The minimum temperatures determined in Antoine equation for most of chemicals used in this study except *n*-heptane are higher than 15 °C. Thus, the calculated saturated vapor pressures at 15 °C as well as the saturated vapor pressures based on the minimum temperature are listed with and without parentheses, respectively, in Table 1 in main text.

Supplementary Figures

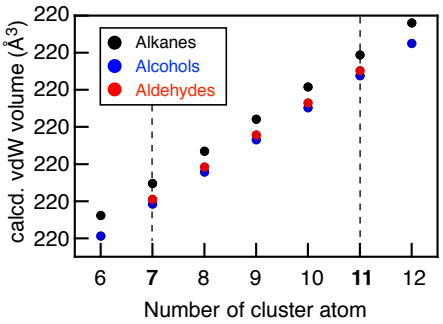

Fig. S1. Calculated van der Waals volume using modified calculation method based on Bondi radii.[1,2] Details can be found in Supplementary Notes in this ESI†.

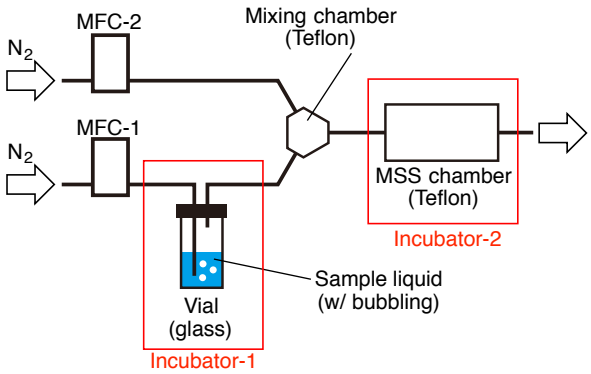

Fig. S2. Schematic illustrations of the measurement system.

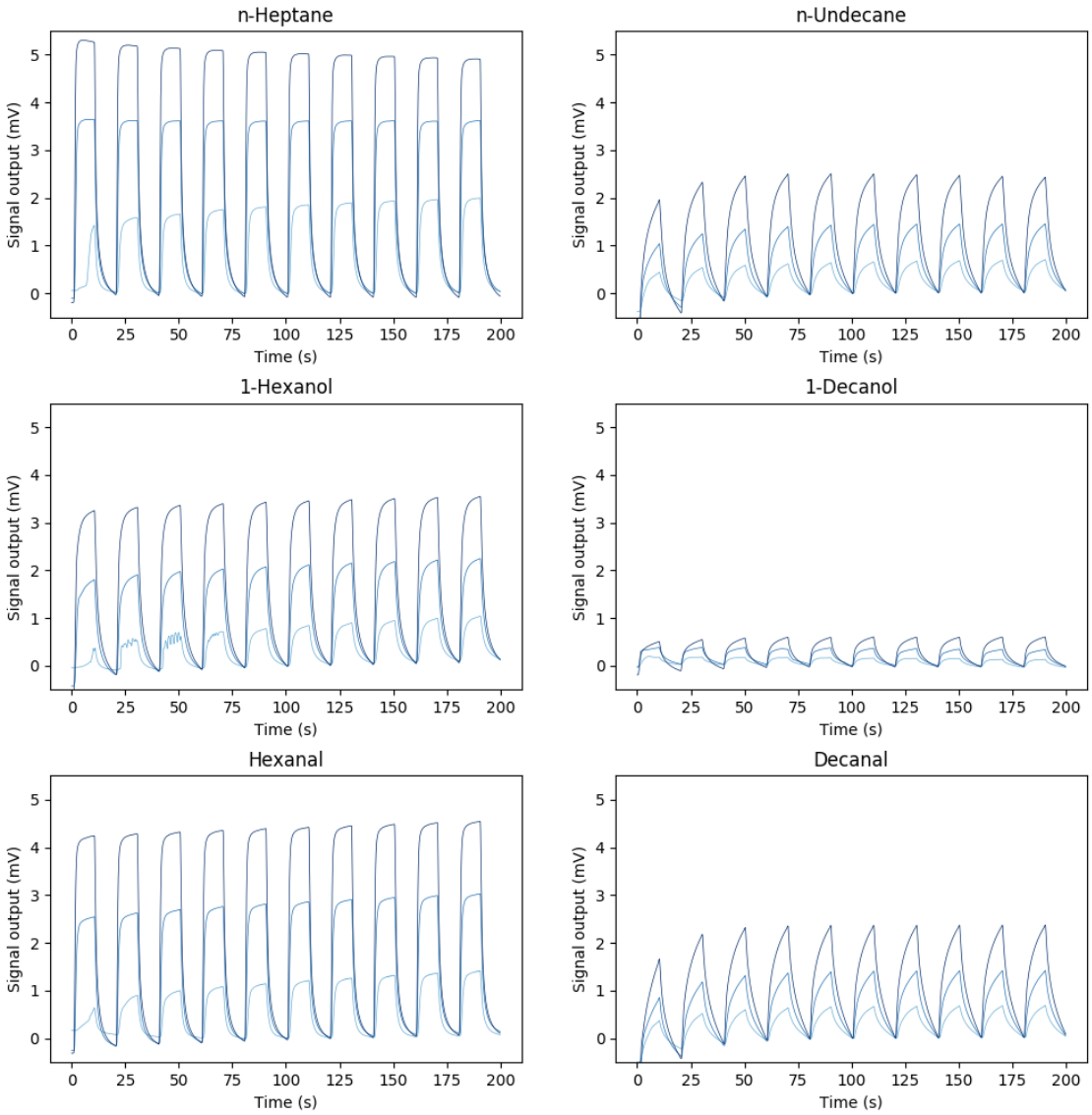

Fig. S3. The whole sensor responses from the vapors of the structurally similar chemicals. Lighter to darker color map indicates P_a / P_o of 0.02, 0.05 and 0.1, respectively; where P_a and P_o stand for partial pressure and saturated vapor pressure of each sample, respectively.

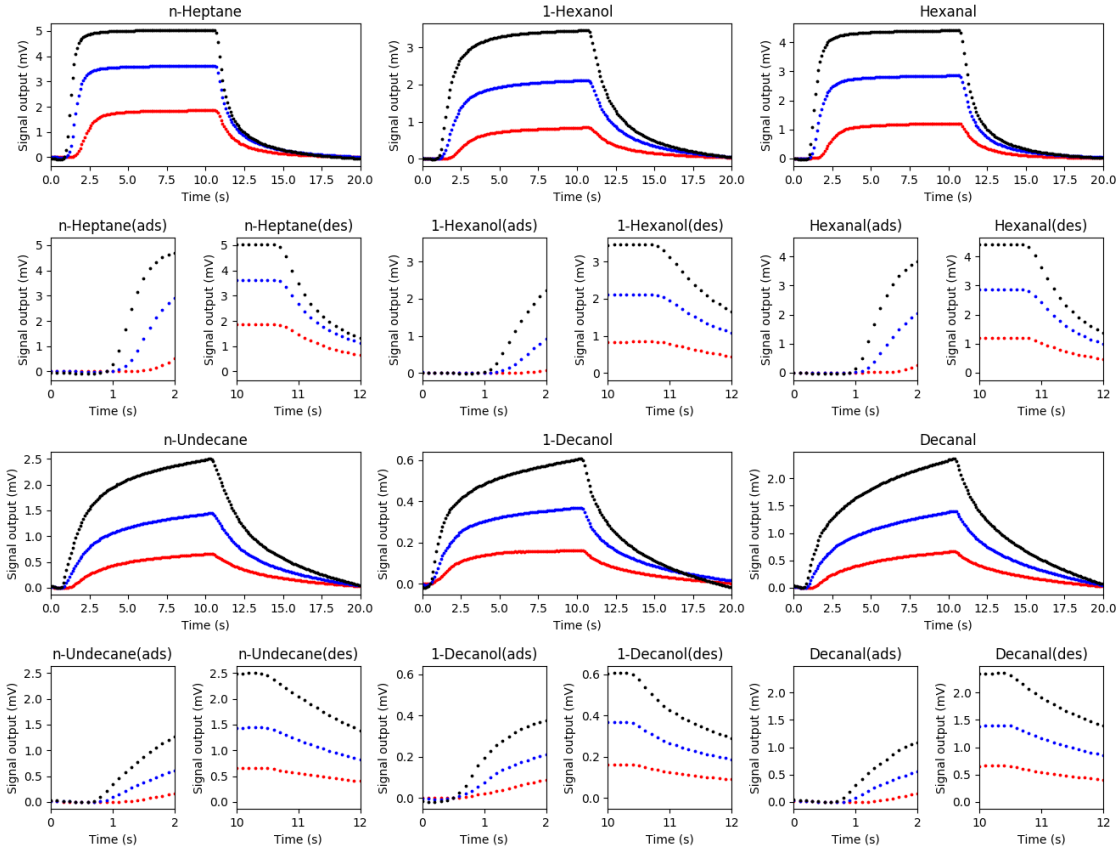

Fig. S4. Signal responses of all chemicals measured in this study. One signal response cycle and enlarged signals at the beginnings of adsorption and desorption.

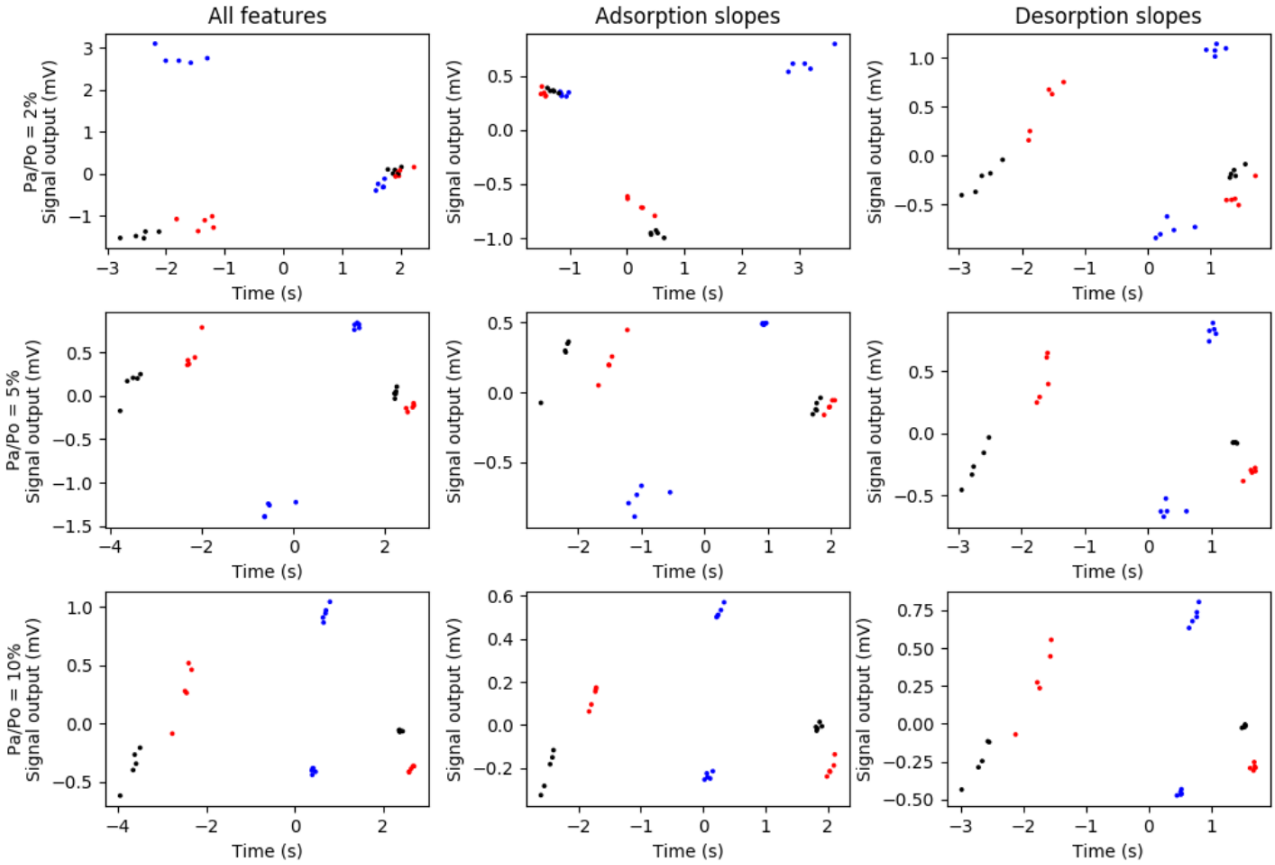

Fig. S5. PCA score plots of all concentration.

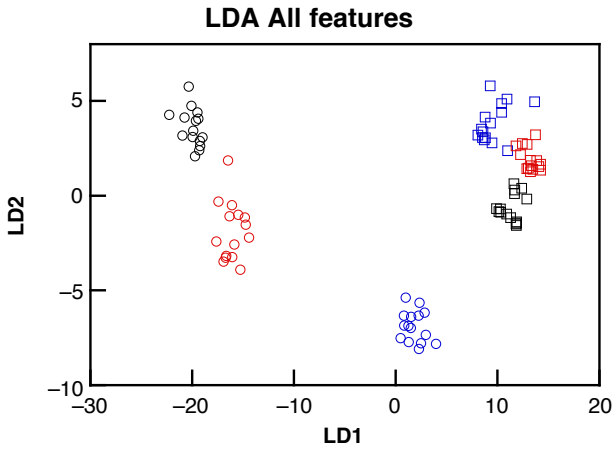

Fig. S6. Linear Discriminant Analysis (LDA).

Supplementary Tables

Table S1. The constant A–C of each chemical for Antoine equation.

Chemicals	A	B	C	Temperature range (°C)
***n*-Heptane**	7.04670	1341.8887	223.733	–1.81 – 123.47
1-Hexanol	7.36642	1544.6108	187.498	55.12 – 181.62
Hexanal	7.16510	1471.3075	214.570	24.08 – 154.8
***n*-Undecane**	7.18058	1706.2645	200.897	75.17 – 225.80
1-Decanol	7.94534	2145.9319	191.869	117.11 – 258.63
Decanal	7.73752	1974.3112	197.962	95.07 – 235.41

Supplementary References

1. A. Bondi, *J. Phys. Chem.,* 1964, **68**, 441–451.
2. Y. H. Zhao, M. H. Abraham, and A. M. Zissimos, *J. Org. Chem.,* 2003, **68**, 7368–7373.
3. C. C. Yaws, *The Yaws Handbook of Vapor Pressure, Antoine Coefficients*, 2nd Edition, (Springer, New York), 2015.