



Leibniz Institute for  
Food Systems Biology  
at the Technical University of Munich

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# The Leibniz-LSB@TUM Odorant Database

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Veronika Mall, Petra Steinhaus

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**COST Action 18225 WaterTOP**  
**Prague, CZ – 19-20 April 2022**

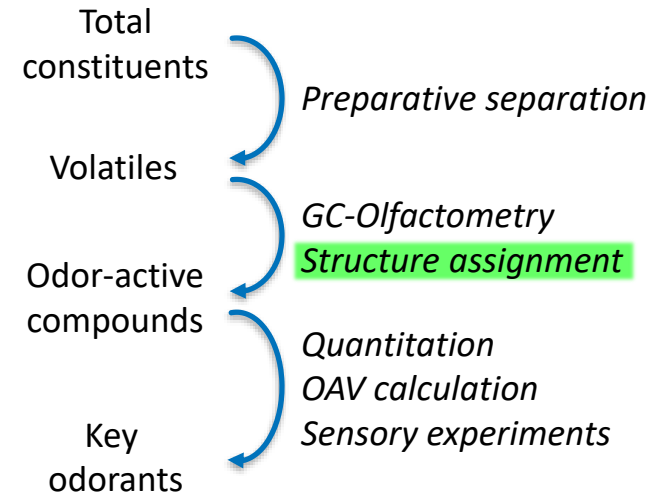
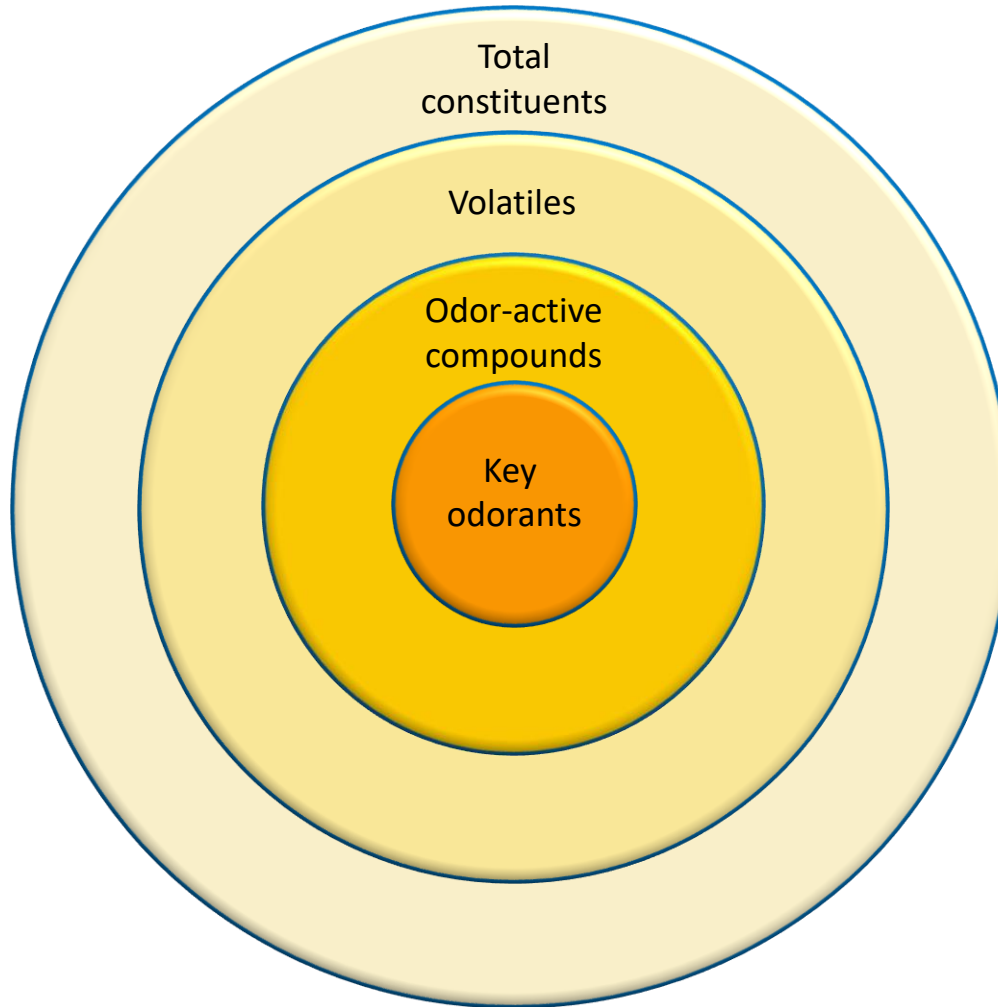


## Target user groups

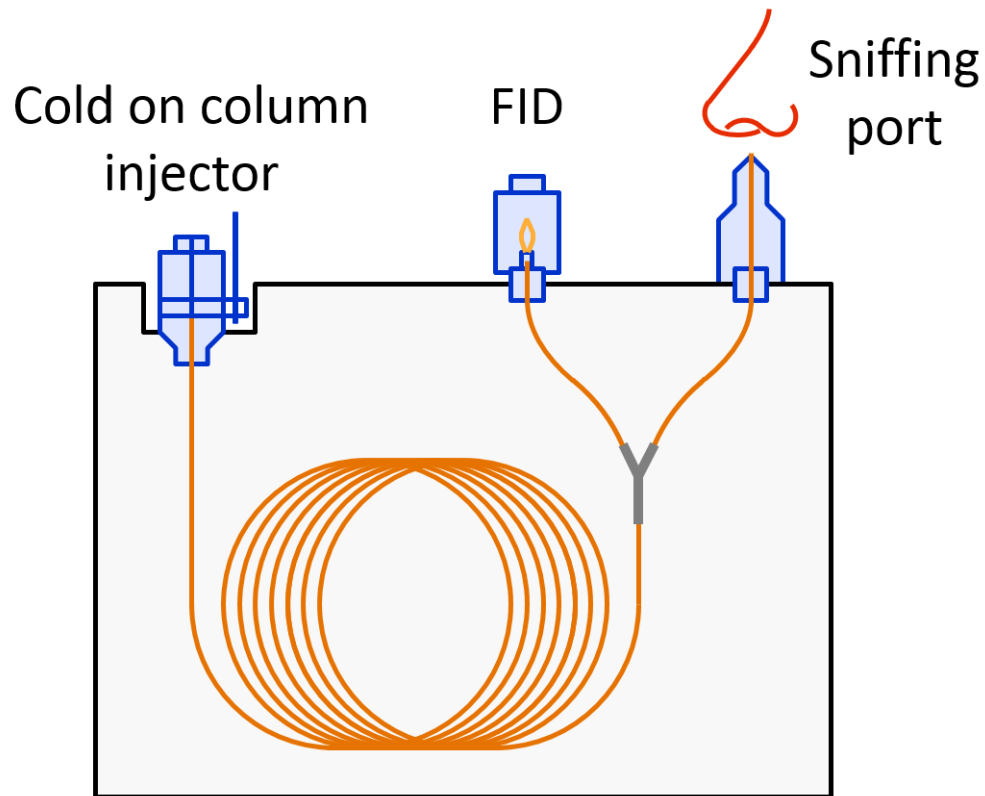
- Researchers applying GC-O to identify odor-active compounds
- Researchers aiming at an approximation of the odor impact of compounds by odor activity value calculations

## Associated key content

- Odor qualities (odor descriptions) and retention indices of odorants on different, widely used GC stationary phases such as DB-5 and FFAP
- Odor threshold values of odorants in different matrices such as water, oil, and hydroalcoholic solutions

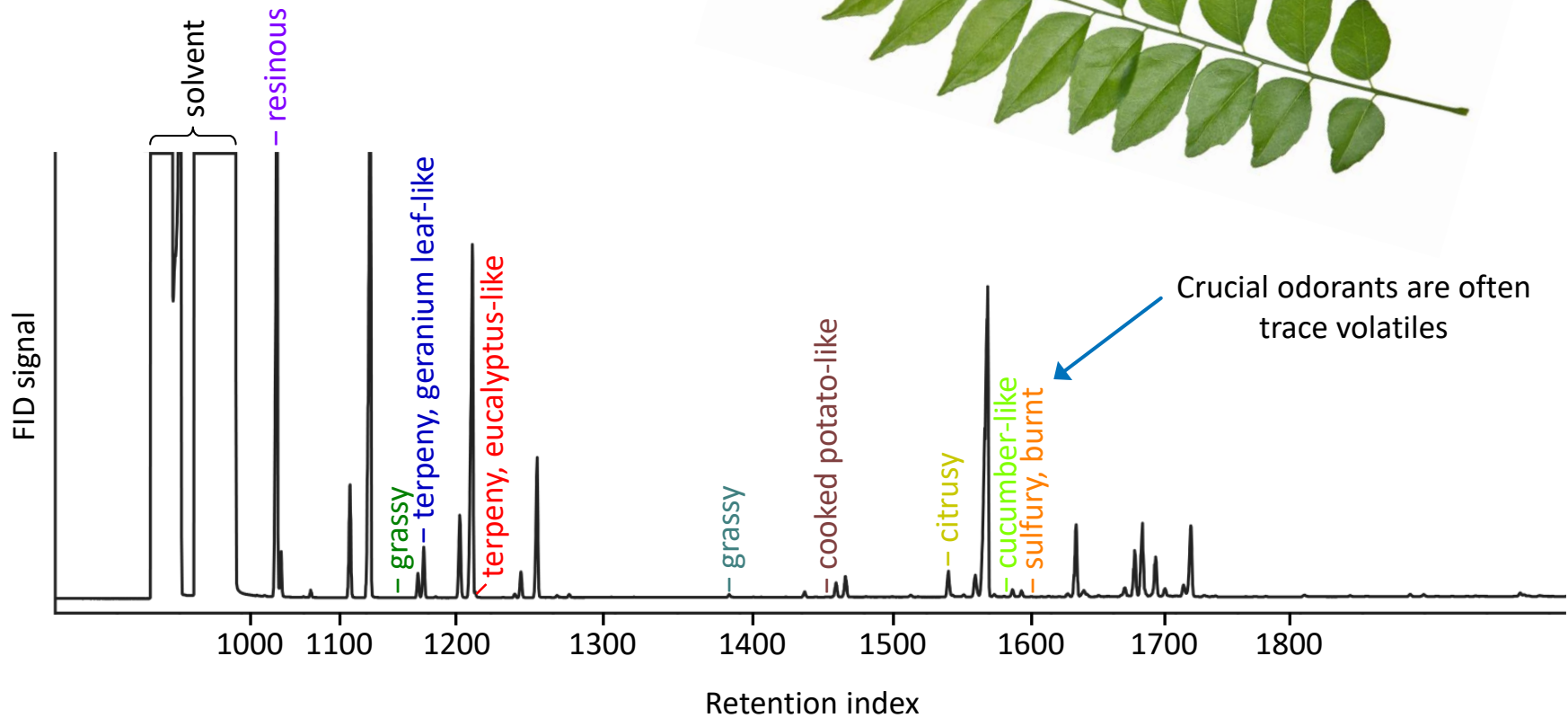


## Gas Chromatography-Olfactometry (GC-O)



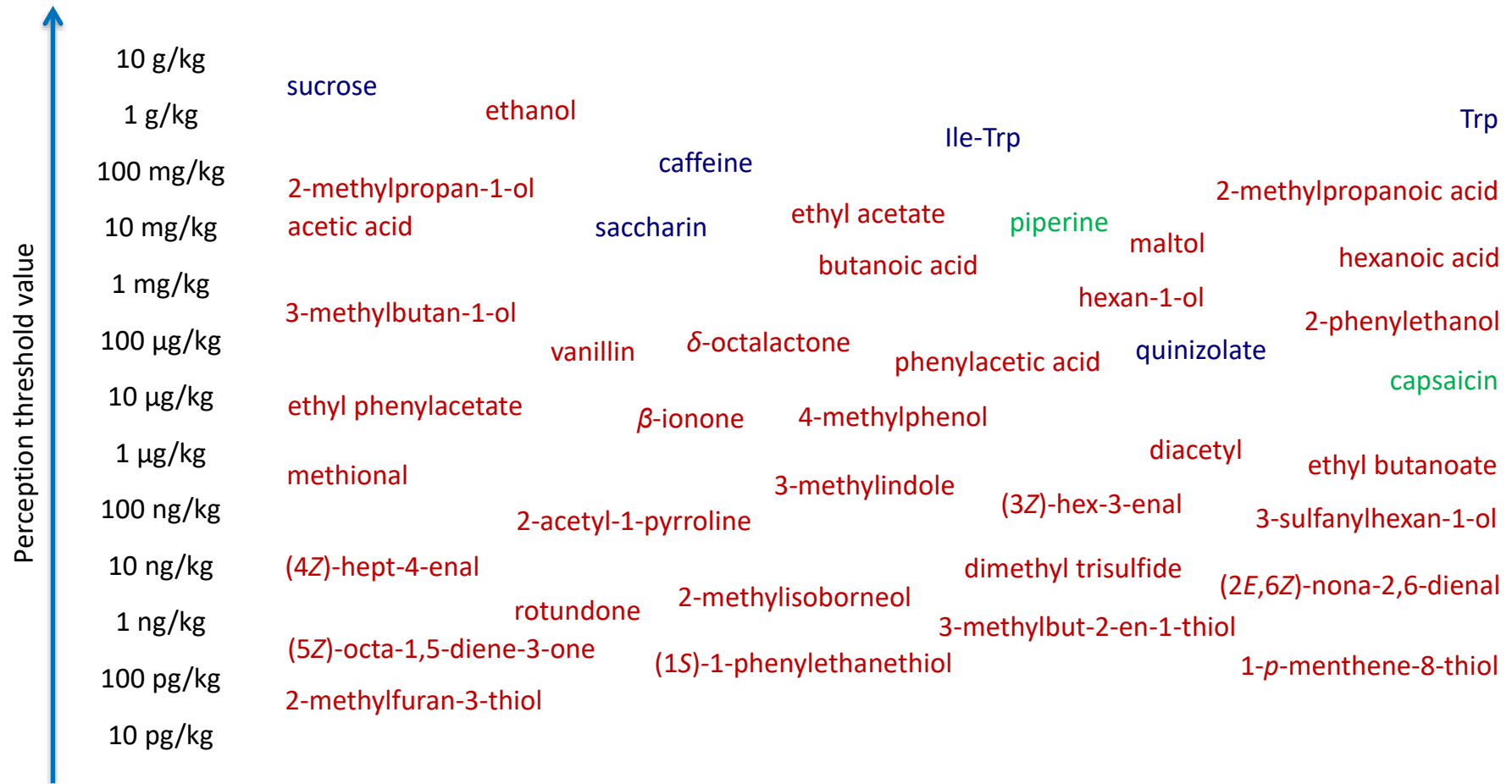
# ACTIVITY-GUIDED ODORANT SCREENING

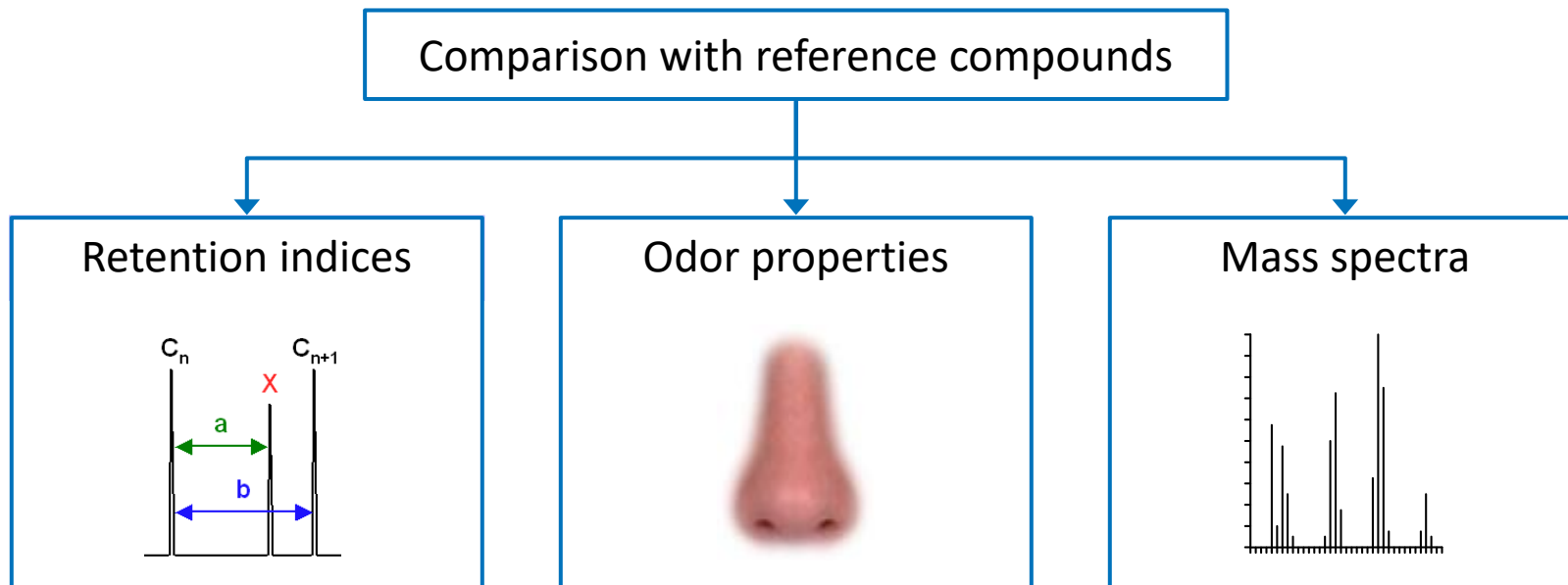




# PERCEPTION THRESHOLD VALUES OF SENSORY ACTIVE COMPOUNDS

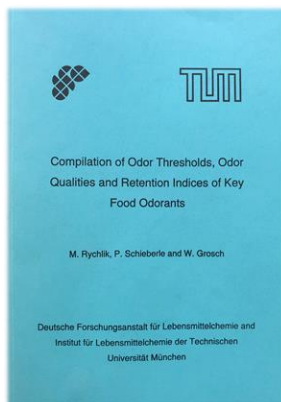
Thresholds of typical food **odorants**, **tastants**, and **chemesthetic agents** in water



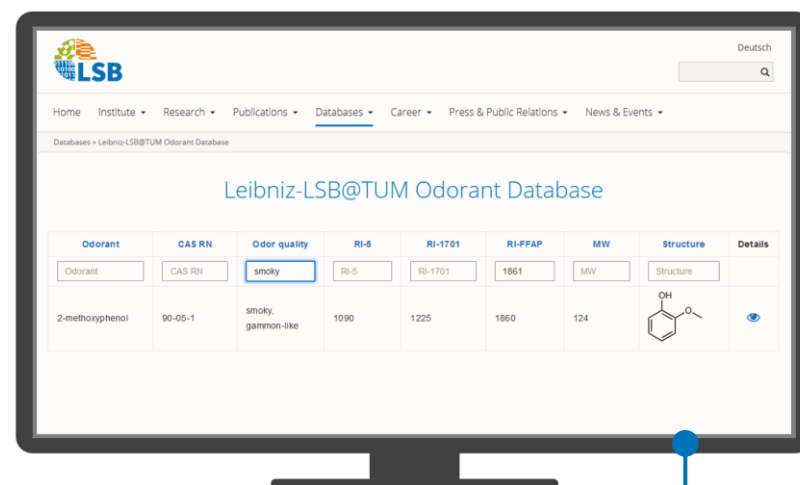


- Preliminary structure assignment by RI and odor is the first choice; it is fast and easy, but requires an elaborate compilation of reliable data
- Unequivocal structure assignment essentially requires analysis of reference compounds (by both, GC-O and GC-MS)

# THE LEIBNIZ-LSB@TUM ODORANT DATABASE: HISTORY



| Nr.  | Aromastoff          | CAS-Nr.  | Geruchsqualität   | RI <sub>5</sub> | RI <sub>1701</sub> | RI <sub>FFAP</sub> |
|------|---------------------|----------|-------------------|-----------------|--------------------|--------------------|
| 0143 | Ethanol             | 64-17-5  | ethanolisch       |                 |                    | 930                |
| 0145 | 2-Methyl-1-propanol | 78-83-1  | Malz              | 646             |                    | 1102               |
| 0319 | 2-Methylpropansäure | 79-31-2  | Schweiß, Käse     | 789             | 964                | 1557               |
| 0036 | Ethylacetat         | 141-78-6 | Lösungsmittel     | 633             | 683                | 891                |
| 0067 | Pentansäure         | 109-52-4 | Schweiß, fruchtig | 914             | 1084               | 1726               |
| 0123 | Propansäure         | 79-09-4  | sauer, schweißig  | 836             | 885                | 1538               |
| 0317 | Essigsäure          | 64-19-7  | Essig             | 610             | 795                | 1443               |
| 0474 | Maltol              | 118-71-8 | Karamell          | 1110            |                    | 1974               |
| 0028 | Hexansäure          | 142-62-1 | Schweiß           | 1018            | 1186               | 1836               |
| 0641 | Phenol              | 108-95-2 | Tinte, phenolisch | 943             |                    | 1995               |
| 0027 | Buttersäure         | 107-92-6 | Schweiß           | 821             | 991                | 1620               |



1995

2000

2020

Cardbox

Booklet

Word tables

Excel tables

HTML tables

Open access



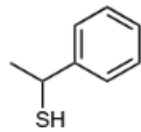
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Datenbanken » Leibniz-LSB@TUM Odorant Database

## Leibniz-LSB@TUM Odorant Database

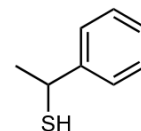
| Odorant                              | CAS RN                                  | Odor quality                      | RI-5                              | RI-1701                             | RI-FFAP                           | MW                              | Structure                                                                            | Details                                                                              |
|--------------------------------------|-----------------------------------------|-----------------------------------|-----------------------------------|-------------------------------------|-----------------------------------|---------------------------------|--------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
| <input type="text" value="Odorant"/> | <input type="text" value="CAS RN"/>     | <input type="text" value="burn"/> | <input type="text" value="RI-5"/> | <input type="text" value="RI-170"/> | <input type="text" value="160C"/> | <input type="text" value="MW"/> | <input type="text" value="Structure"/>                                               |                                                                                      |
| 1-phenylethanethiol                  | 6263-65-6,<br>33877-16-6,<br>33877-11-1 | burned                            | 1120                              | 1214                                | 1599                              | 138                             |  |  |

## Leibniz-LSB@TUM Odorant Database

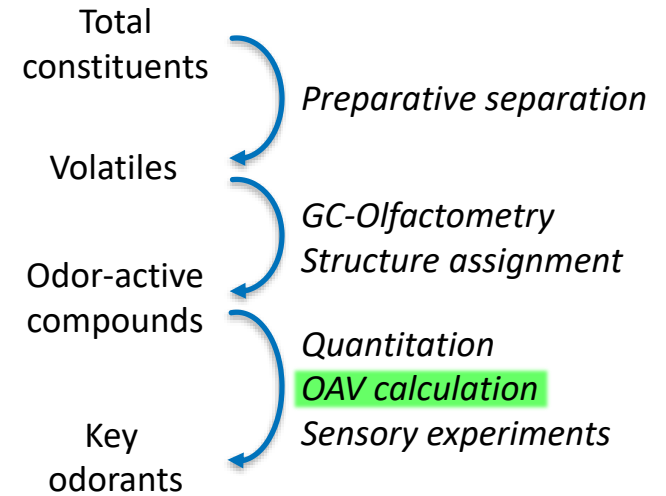
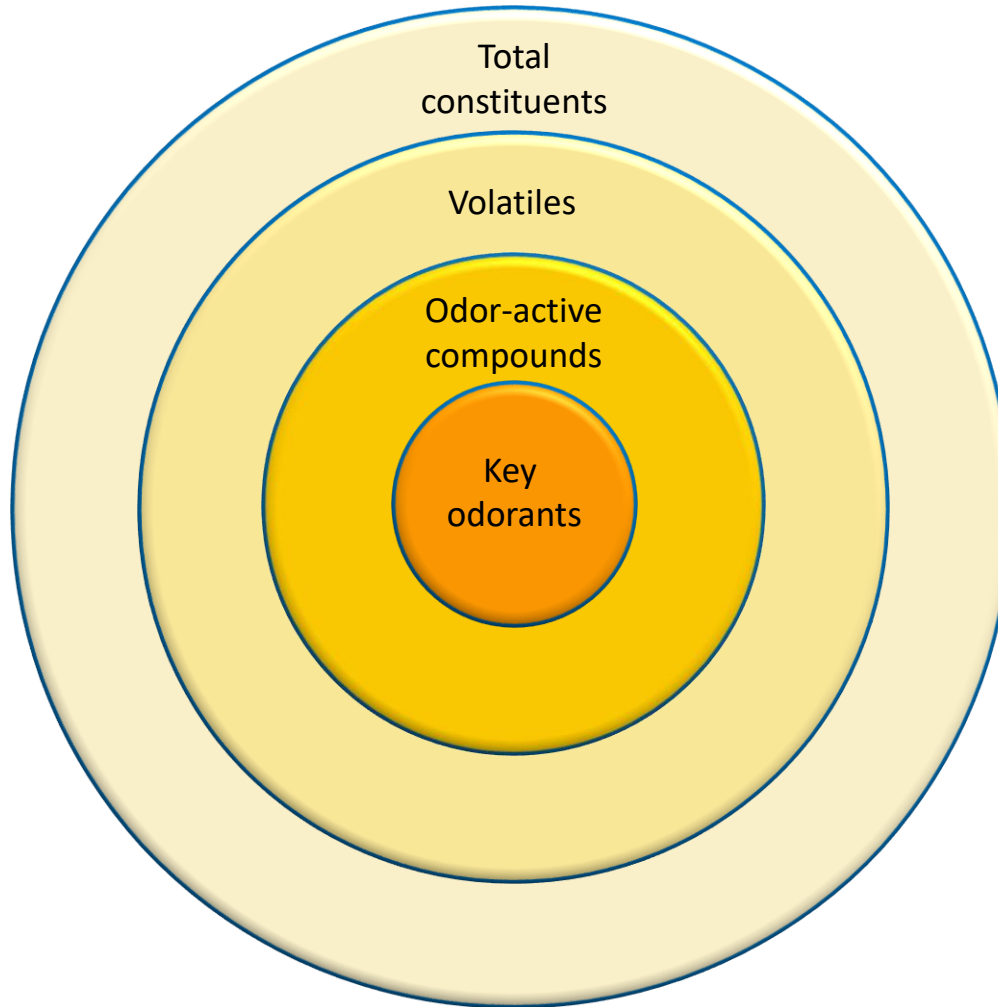
### Substance details

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#### 1-phenylethanethiol



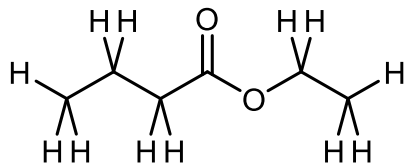
| Reference                                                                                                                                                                                                                                                                                               | Year | Occurrence         | Odor quality                     | Odor threshold                                                           | RI-1 | RI-5 | RI-1701 | RI-FFAP | RI-WAX | Synthesis |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|--------------------|----------------------------------|--------------------------------------------------------------------------|------|------|---------|---------|--------|-----------|
| Reference                                                                                                                                                                                                                                                                                               | Year | Occurrence         | Odor quality                     | Odor threshold                                                           | RI-1 | RI-5 | RI-1701 | RI-FFAP | RI-WAX | Synthesis |
| Fischer A, Grab W, Schieberle P (2008) Eur Food Res Technol 227: 735-744, DOI: 10.1021/jf801070r. Characterisation of the most odour-active compounds in a peel oil extract from Pontianak oranges (Citrus nobilis var. Lour. Microcarpa Hassk.)                                                        | 2008 | orange peel oil    | sulfury, resin-like              |                                                                          |      | 1116 | 1214    | 1592    |        |           |
| Fischer A, Schieberle P (2009) Eur Food Res Technol 229: 319-328, DOI: 10.1007/s00217-009-1058-4. Characterization of the key aroma compounds in the peel oil of Pontianak oranges (Citrus nobilis Lour. Var. microcarpa Hassk.) by aroma reconstitution experiments                                    | 2009 | orange peel oil    |                                  |                                                                          |      |      |         |         |        | ✓(d5)     |
| Steinhaus M (2015) J Agric Food Chem 63: 4060-4066, DOI: 10.1021/acs.jafc.5b01174. Characterization of the major odor-active compounds in the leaves of the curry tree Bergera koenigii L. by aroma extract dilution analysis                                                                           | 2015 | curry leaf         | sulfury, burnt                   |                                                                          |      | 1120 |         | 1601    |        |           |
| Steinhaus M (2017) J Agric Food Chem 65: 2141-2146, DOI: 10.1021/acs.jafc.7b00197. Confirmation of 1-phenylethane-1-thiol as character impact aroma compound in curry leaves and its behavior during tissue disruption, drying, and frying                                                              | 2017 | curry leaf         |                                  | (S) OT-water 0.00021 µg/kg;<br>(R) OT-water 0.00054 µg/kg                |      |      |         |         |        |           |
| Schoenauer S, Buergy A, Kreissl J, Schieberle P (2019) J Agric Food Chem 67: 2598-2606, DOI: 10.1021/acs.jafc.9b00353. Structure/odor activity studies on aromatic mercaptans and their cyclohexane analogues synthesized by changing the structural motifs of naturally occurring phenyl alkaneethiols | 2019 |                    | sulfury, burned, curry leaf-like | (rac) OT-air 0.0010 ng/L; (R) OT-air 0.032 ng/L; (S) OT-air 0.00025 ng/L |      | 1123 |         | 1591    |        | ✓         |
| Marcinkowska M, Frank S, Steinhaus M, Jeleń HH (2021) J. Agric. Food Chem. 69: 12270–12277. DOI: 10.1021/acs.jafc.1c04339. Key odorants of raw and cooked green kohlrabi (brassica oleraceavar. gongylodes L.)                                                                                          | 2021 | raw green kohlrabi | burned                           |                                                                          |      | 1122 |         | 1626    |        |           |



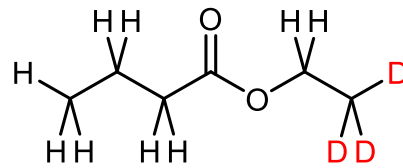
# ODORANT QUANTITATION: STABLE ISOTOPE DILUTION ANALYSIS (SIDA)

**Concept:** A stable isotopically substituted analogue **S** of the analyte **A** is added to the sample prior to the workup as an internal standard

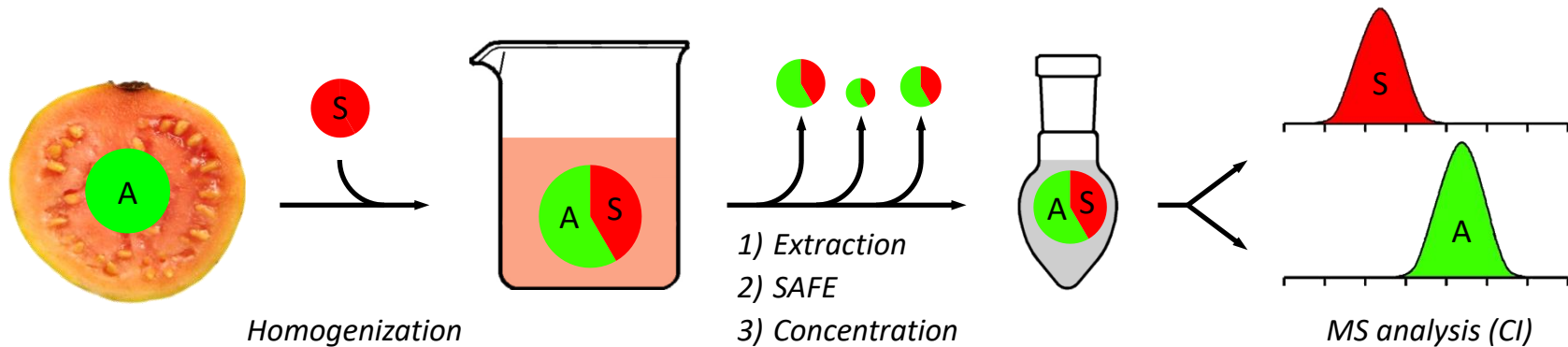
**Example:**



**Analyte:** Ethyl butanoate



**Standard:** (2,2,2-<sup>2</sup>H<sub>3</sub>)Ethyl butanoate



**Pro:** Any loss of the analyte is fully compensated, because the standard is behaving in an identical way under the conditions of a mild workup

**Con:** For each analyte an individual standard is required

# CONCENTRATIONS AND OAVS OF GUAVA ODORANTS

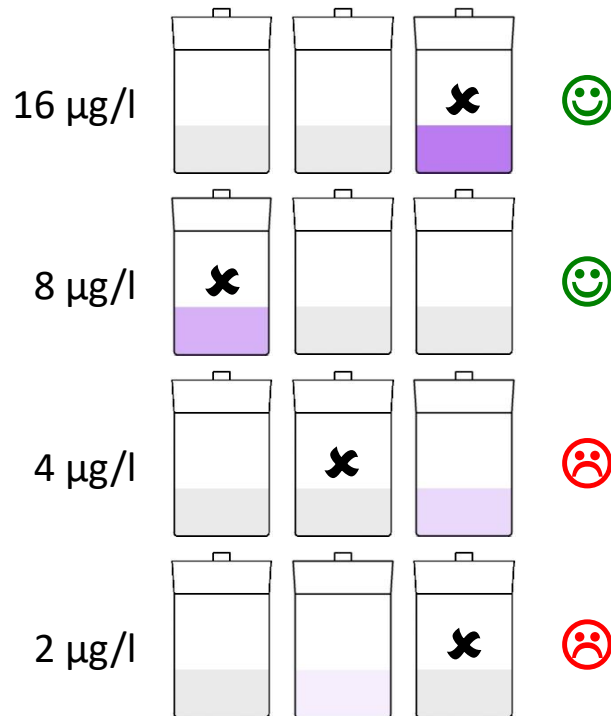
| Compound                                    | Concentration<br>(µg/kg) | Odor threshold<br>(µg/kg) | OAV   |
|---------------------------------------------|--------------------------|---------------------------|-------|
| acetaldehyde                                | 2400                     | 25                        | 98    |
| (3Z)-hex-3-enal                             | 1600                     | 0.12                      | 14000 |
| 4-hydroxy-2,5-dimethylfuran-3(2H)-one       | 1400                     | 40                        | 36    |
| cinnamyl acetate                            | 1300                     | 150                       | 5.7   |
| cinnamyl alcohol                            | 860                      | 77                        | 17    |
| hexanal                                     | 650                      | 2.4                       | 360   |
| (R/S)-3-sulfanylhexas-1-ol                  | 560                      | 0.06                      | 9300  |
| ethyl butanoate                             | 130                      | 0.76                      | 170   |
| methyl (2S,3S)-2-hydroxy-3-methylpentanoate | 27                       | 2.4                       | 11    |
| <i>trans</i> -4,5-epoxy-(2E)-dec-2-enal     | 17                       | 0.22                      | 76    |
| (R/S)-3-sulfanylhexyl acetate               | 11                       | 0.02                      | 570   |
| methyl (2R,3S)-2-hydroxy-3-methylpentanoate | 9.7                      | 13                        | 0.7   |
| 4-methoxy-2,5-dimethylfuran-3(2H)-one       | 9.4                      | 160                       | <<1   |
| ethyl benzoate                              | 7.2                      | 53                        | <<1   |
| sotolon                                     | 4.3                      | 1.7                       | 2.5   |
| methyl benzoate                             | 2.6                      | 73                        | <<1   |
| methional                                   | 1.3                      | 0.43                      | 3.1   |

# CONCENTRATIONS AND OAVS OF GUAVA ODORANTS

| Compound                                                      | Concentration<br>( $\mu\text{g/kg}$ ) | Odor threshold<br>( $\mu\text{g/kg}$ ) | OAV   |
|---------------------------------------------------------------|---------------------------------------|----------------------------------------|-------|
| (3Z)-hex-3-enal                                               | 1600                                  | 0.12                                   | 14000 |
| (R/S)-3-sulfanylhexas-1-ol                                    | 560                                   | 0.06                                   | 9300  |
| (R/S)-3-sulfanylhexasyl acetate                               | 11                                    | 0.02                                   | 570   |
| hexanal                                                       | 650                                   | 2.4                                    | 360   |
| ethyl butanoate                                               | 130                                   | 0.76                                   | 170   |
| acetaldehyde                                                  | 2400                                  | 25                                     | 98    |
| <i>trans</i> -4,5-epoxy-(2 <i>E</i> )-dec-2-enal              | 17                                    | 0.22                                   | 76    |
| 4-hydroxy-2,5-dimethylfuran-3(2 <i>H</i> )-one                | 1400                                  | 40                                     | 36    |
| cinnamyl alcohol                                              | 860                                   | 77                                     | 17    |
| methyl (2 <i>S</i> ,3 <i>S</i> )-2-hydroxy-3-methylpentanoate | 27                                    | 2.4                                    | 11    |
| cinnamyl acetate                                              | 1300                                  | 150                                    | 5.7   |
| methional                                                     | 1.3                                   | 0.43                                   | 3.1   |
| sotolon                                                       | 4.3                                   | 1.7                                    | 2.5   |
| methyl (2 <i>R</i> ,3 <i>S</i> )-2-hydroxy-3-methylpentanoate | 9.7                                   | 13                                     | 0.7   |
| ethyl benzoate                                                | 7.2                                   | 53                                     | <<1   |
| 4-methoxy-2,5-dimethylfuran-3(2 <i>H</i> )-one                | 9.4                                   | 160                                    | <<1   |
| methyl benzoate                                               | 2.6                                   | 73                                     | <<1   |

Method: ASTM E679-19 standard practice for determination of odor and taste thresholds by a forced-choice ascending concentration series method of limits

Example:



Individual odor threshold:

$$T_i = \sqrt{4 \mu\text{g/l} \times 8 \mu\text{g/l}}$$

Averaged odor threshold:

$$\bar{T} = \sqrt[n]{\prod_{i=1}^n T_i}$$

Crucial point to obtain comparable and reliable data: Avoid confirmation bias by ...

- ... following a strict protocol
- ... using a test supervisor and a panel not involved in the research project

Eur Food Res Technol (2008) 228:265–273  
DOI 10.1007/s00217-008-0931-x

ORIGINAL PAPER

## Re-investigation on odour thresholds of key food aroma compounds and development of an aroma language based on odour qualities of defined aqueous odorant solutions

Michael Czerny · Martin Christlbauer · Monika Christlbauer ·  
Anja Fischer · Michael Granvogl · Michaela Hammer ·  
Cornelia Hartl · Noelia Moran Hernandez · Peter Schieberle

Received: 20 May 2008 / Revised: 10 July 2008 / Accepted: 17 July 2008 / Published online: 5 August 2008  
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**Abstract** Literature data on odour thresholds of volatile food constituents, and, in particular on their odour quality, may differ significantly. In order to obtain more reliable sensory data, the odour thresholds of eighty-four com-

because it is believed that the whole set of volatiles present in a given food interacts with the human odorant receptors, thus generating a certain odour profile in the brain.

It may be true that the human odorant receptors are able